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Fractional Partial Differential Equations for Conservation Laws and Beyond: Theory, Numerics, and Applications (Summary Technical Report, Sep 2015–Nov 2022)

by Joseph Myers

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Fractional Partial Differential Equations for Conservation Laws and Beyond: Theory, Numerics, and Applications (Summary Technical Report, Sep 2015–Nov 2022)

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14. ABSTRACT The FY15 Multidisciplinary University Research Initiative topic “Fractional PDEs for Conservation Laws and Beyond: Theory, Numerics, and Applications” led by Professor George Karniadakis at Brown University was active from 16 September 2015 through 29 November 2022. The objective of the effort has been to develop a new rigorous theoretical and computational framework enabling end-to-end fractional-order modeling of physical problems governed by conservation laws in large-scale simulations. Progress in the development of these fractional-order methods hold promise for more accurate modeling and prediction in systems involving unobserved processes or systems where the physics is not well-understood.			
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1. Introduction

The FY15 Multidisciplinary University Research Initiative (MURI) topic titled “Fractional Partial Differential Equations (aka FPDEs) for Conservation Laws and Beyond: Theory, Numerics, and Applications” led by Professor George Karniadakis at Brown University was active from 16 September 2015 through 22 November 2022. The objective of the effort has been to further our understanding and modeling capabilities in situations where there may be unknown or unobserved processes—where there is memory, where there is a time lag between cause and effect, where the time history has an effect on system evolution, and others—by developing understanding, methods, and tools in the area of fractional operators, as well as to develop a new rigorous theoretical and computational framework enabling end-to-end fractional modeling of physical problems governed by conservation laws in large-scale simulations. This involves new results in the theory of FPDEs (where we understand PDEs, or Partial Differential Equations, to mean equations that involve several smoothly varying independent factors that together determine the output), data-driven construction of solutions to this class of data-dense operators, benchmark examples, new models for turbulence and multiphase systems, and distribution to the community through open source code.

To a large extent, much of engineering design is built on the tools of calculus, where things are assumed to happen instantaneously at a given point. The result is effects limited to a point in space and to a vanishingly small instant in time. Problems arise when trying to apply these tools to unobserved/unmeasured processes, or to processes involving mixing, anomalous diffusion, surface ablation, wear, memory effects, and others. These classical models often do a poor job of describing observations of process in those situations; one should be wary of any model that needs to include anomalous *anything* to describe observations. Therefore this investigation looks further, to classes of operators that are not local (in the sense of the vanishingly small limits of calculus) but rather are nonlocal. So the objectives of this effort have been to accomplish the following:

- 1) Identify mathematical constructs that are not based on local operators, but rather admit nonlocality to analyze processes and use these as the basis for new models.
- 2) Develop computational methods for solving these new types of equations.
- 3) Demonstrate the validity of the methods in the context of an application that is important to the Army.

Action: The first step down this path was for me as Program Manager (PM) to suggest and sponsor an invited conference in this area; this conference was held in Newport, Rhode Island, in 2015 and attracted mathematicians from across the United States and Europe. Based on presentations there and follow-on discussions, our Fluid Dynamics PM (Munson) and I teamed up to author this MURI topic in the area. The winning team was headed by Brown University (Professor George Karniadakis) and included Michigan State, Columbia, University of South Carolina, and Rice. The project, Fractional PDEs for Conservation Laws and Beyond: Theory, Numerics, and Applications, focused on developing nonlocal operators, which by definition allow both action at a distance and (causal) memory effects. After the first couple of reviews, we arranged for the annual reviews to be conducted at the US Army Combat Capabilities Command (DEVCOM) Army Research Laboratory (ARL) with the (then) Vehicle Technology Directorate (now redesignated into the Weapons and Materials Research and Development Directorate), Dr Anindya Ghoshal's group. We arranged all future reviews to be conducted there (first in person and later virtually). This was very productive in not only sharing advances from the academic team with laboratory personnel, but also after a couple of years of work and initial successes, enabling the academic team to share with the government team their newly developed solver for Physics-Inspired Neural Networks (PINNS).

2. Overview of Results

It turns out that one of the challenges involved in solving fractional-order PDEs is in applying correct and consistent conditions at the boundaries; the PIs have been able to develop a new computational method, Physics INspired Neural Networks (PINNS), to determine the fractional operator order based solely on boundary data, requiring no other derivative data (Fig. 1). This is a significant advance; it greatly simplifies numerical solutions of these FPDEs with significantly more accuracy.

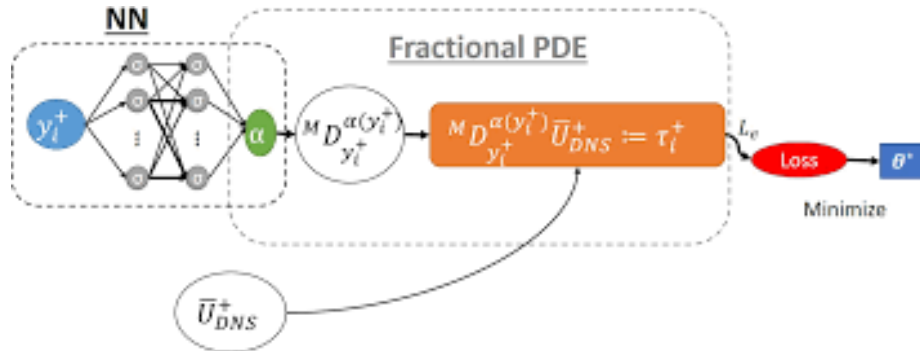


Fig. 1 Fractional PINNs discover variable fractional order in turbulence

Success Summary: A new type of calculus has been developed that can incorporate the influence of unseen dynamics, and new computational methods have been developed that are enabling new models that more accurately describe and predict the evolution of systems with memory or other unseen processes. These more robust and accurate tools, and these developments of new types of mathematical operators, are developing best-in-world capability for high-fidelity fluid-structure interaction design and wear resistance, as now being applied in ARL–Weapon Sciences (WS) turbine applications and others.

Future Capability: This new class of modeling capability will replace many existing models that require both full knowledge and deterministic physics with models that are still physics-based but which also account for unobserved lower-level processes.

New features and impacts of this work include the following:

- New computational methods have been developed that replace the limiting processes of calculus with a more far-seeing domain; these have enabled models that more accurately describe and predict the evolution of systems with memory or with otherwise unaccounted-for subprocesses.
- These new operators, incorporating PINNS, have demonstrated ability for higher-fidelity modeling in the presence of anomalous transport, non-Markovian behavior and long-range interactions, self-similarity and scaling, singular behavior, interfaces, and finite-domain decorrelation effects.
- ARL-WS (Luis Bravo and Anindya Ghoshal) are now applying these tools to ARL–WS turbine applications and have achieved higher fidelity fluid-structure interaction/wetting design, enabling improved turbine wear monitoring.

3. Knowledge Transitions

The Fractional PDEs for Conservation Laws and Beyond: Theory, Numerics, and Applications MURI has produced more than 250 peer-reviewed journal articles, more than 100 invited and plenary talks, a volume on numerical methods in the *Handbook of Fractional Calculus with Applications, Vol 3: Numerical Methods*, (Walter de Gruyter; 2019), two workshops, and several mini-symposia by the MURI PIs, as well as developed novel software, shared ideas and papers with ARL–WS scientists, and trained 12 new PhDs with placement into new jobs including at Brown and Harvard.

3.1 Publications

- Volume on numerical methods in *Handbook of FPDEs*
- A research monograph on nonlocal modeling
- More than 250 papers published in the six research areas of MURI
- More than 100 invited and plenary talks by MURI scientists
- Two major workshops and several mini-symposia organized by MURI PIs

A complete set of publications is available in the Final Report Appendix.

3.2 Engagements with DOD

PIs Karniadakis, Wang, and Zhen Li met bi-weekly with the research groups of Dr Anindya Ghoshal and Dr Luis Bravo of Propulsion Division, WS, to discuss applications of these methods to the modeling of droplets and wetting in turbines, using dissipative particle dynamics, turbulence modeling, electrostatic modeling, and fractional calculus. Karniadakis' group helped develop work on wall-turbulence fractional models to replace the classical wall functions approach used in laboratory large eddy simulation models. They transferred the code Fractional Physics-Informed Neural Networks (fPINNs) and Dissipative Particle Dynamics (DPD) code to ARL.

PI George Karniadakis (Brown) received a Vannevar Bush Fellowship in 2022 during the course of this DOD-supported research, proposing extensions to the advances of this MURI effort.

Way Ahead: The contact angle at the coating/turbine blade interface is important because it informs about the wettability of the material coating, which is related to blade wear, especially in sandy environments. And so abilities for prediction, engineering design, and control of the contact angle in coatings is practically of great importance. Dr Anindya Ghoshal and Dr Luis Bravo, ARL–WS, are using these methods to formulate predictive tools for exploring the design and wear of heterogeneous functionalized surfaces. This information will then be used to guide the manufacturing of next-generation turbine blade coatings. It is known that a material that exhibits hydrophobicity (a measure of the tendency to orient toward a non-aqueous environment rather than an aqueous environment—a type of “water-repelling”) with respect to sand in the laboratory will likely perform better under engine-relevant conditions. This will be pursued as a design tool for more durable turbine blades and longer-lived performance.

3.3 Software

Karniadakis, Wang, and Zhen Li (add-on) developed the code fPINNs, an open source parallel code for computing the spectral fractional Laplacian on complex geometry.

- fPINNs
- F-NEKTAR++: the first open-source parallel 3-D code for FPDEs

4. DOD Transitions

Members of the MURI helped begin a Small Business Technology Transfer Program with models that are still physics-based but which also account for unobserved lower level processes that developed some of the most general methods from the MURI. They also commercialized the results, to include transferring the fPINNs and DPD codes to ARL (Ghoshal, Bravo, and Geneston, all WS) for use in their work in modeling wetting and wear in turbines.

Appendix. Research Performance Progress Report (RPPR) Final Report

This appendix appears as a pdf attached to the report.

List of Symbols, Abbreviations, and Acronyms

3-D	three-dimensional
ARL	Army Research Laboratory
DEVCOM	US Army Combat Capabilities Development Command
DOD	Department of Defense (US)
DPD	Dissipative Particle Dynamics
FPDE	Fractional Partial Differential Equation
fPINNS	Fractional Physics INspired Neural Networks
FY	fiscal year
MURI	Multi-University Research Initiative
MURI	Multidisciplinary University Research Initiative
PDE	Partial Differential Equation
PINNS	Physics INspired Neural Networks
PM	Program Manager
RPPR	Research Performance Progress Report
WS	Weapons Sciences

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