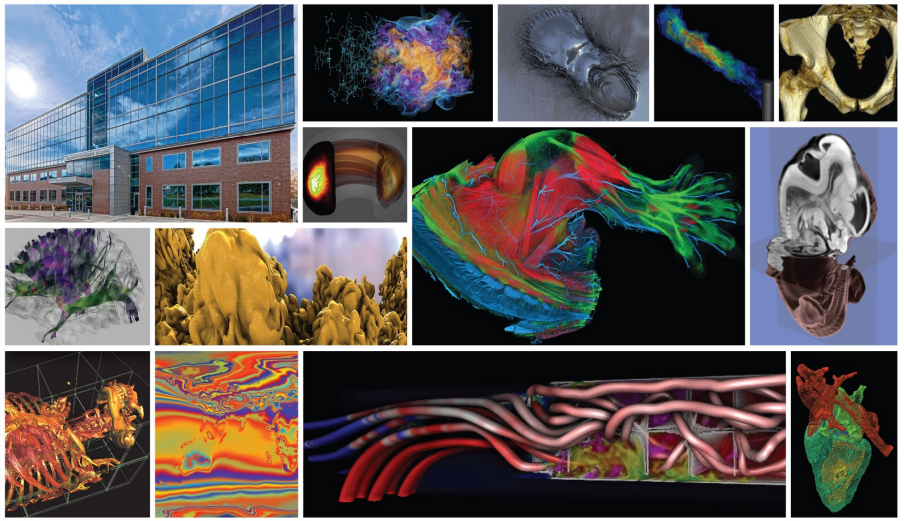
Returning to the Scene of the Crime: Perspective on Translational Computer Science Research

Manish Parashar*

Director, Scientific Computing & Imaging (SCI) Institute

Presidential Professor, School of Computing

University of Utah



CCDSC 2022, Chemin de Chanzé, France

September 07, 2022

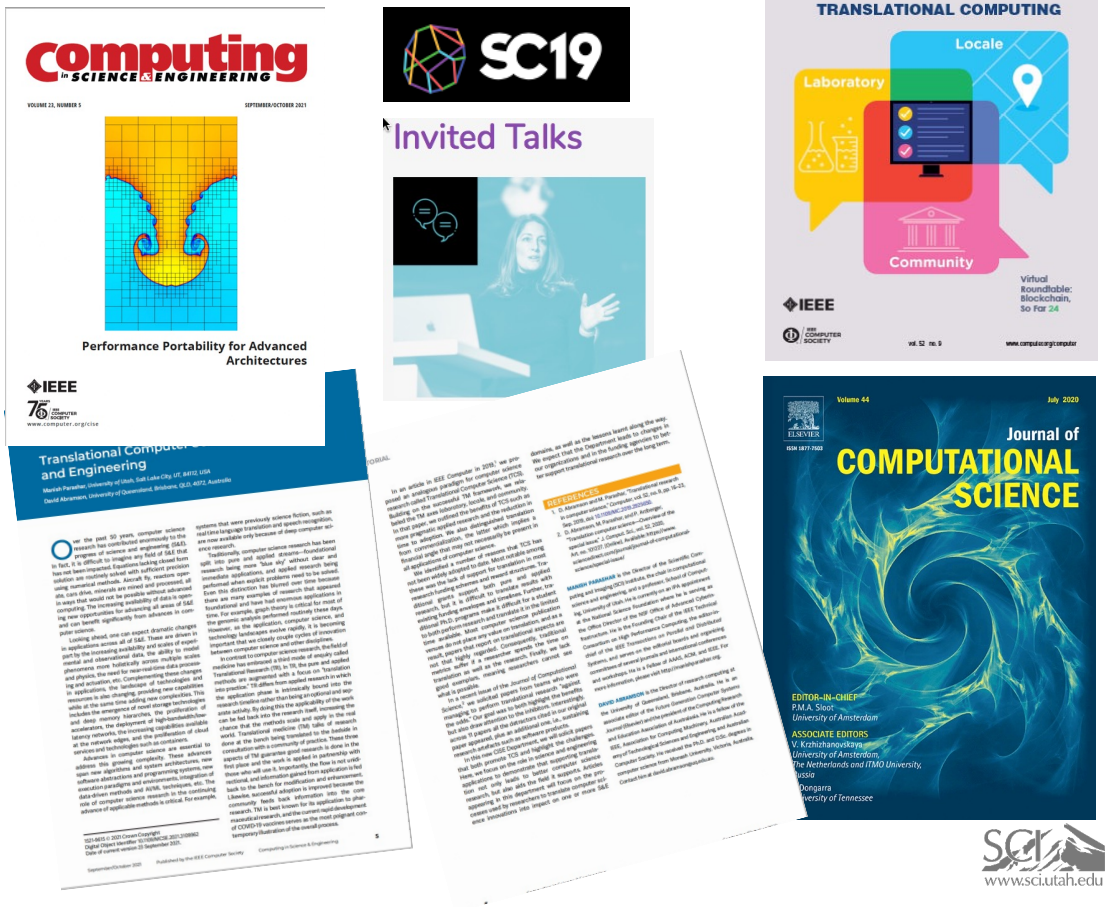
THE UNIVERSITY OF UTAH®

***with David Abramson**

SCI www.sci.utah.edu

The role of a French chateaux and red wine … with David Abramson

Workshop on CCDSC, Lyon France, 2018
Jack Dongarra, Bernard Tourancheau



THE UNIVERSITY OF UTAH®

SCI
www.sci.utah.edu

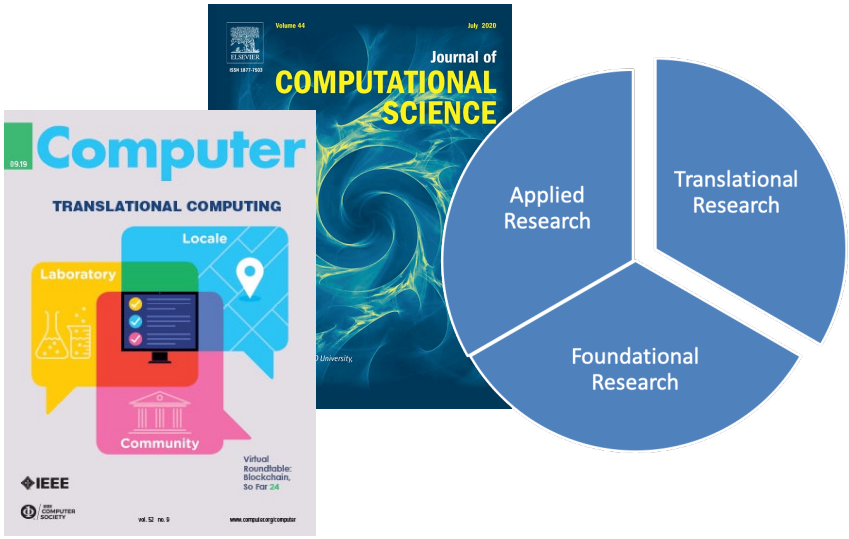
Background: Translational Medicine

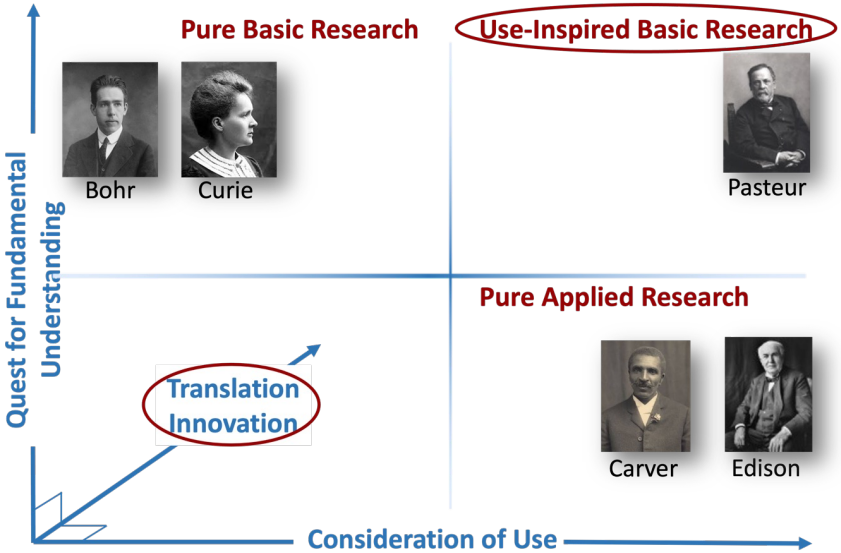
- An interdisciplinary branch of the biomedical field supported by three main pillars:
  - Benchside, Bedside and Community
  - Combines disciplines, resources, expertise, and techniques within these pillars to promote enhancements in prevention, diagnosis, and therapies
- Differs subtly from applied biomedical research, in which a research problem has a potential real-world application
  - Findings are applied as a specific phase of the research plan
  - This not only demonstrates applicability and practicality, but also generates tangible outcomes
- Now well understood and has become a de-facto standard for much of biomedical research
- Intrinsically helps generate outcomes because the research is applied as part of the original plan, as opposed to being an afterthought once the project has completed

Translational Computer Science (TCS)

TCS refers to research that bridges foundational and use-inspired (and applied) research with the *delivery and deployment of its outcomes* to the target community and supports essential *bi-direction interplays* where delivery and deployment process informs the research

- Motivated by the growing importance of computing and data across all of science and society
- Aimed at accelerating the impact of computer, computational and data science
- Inspired by the definition and impact of Translational Medicine
- Focused on taking research from the *Laboratory* to the *Locale* to the *Community*
  - Laboratory, Locale might be physical or virtual
  - Community: Users and early adopters who work with the technology, and can include public bodies that would help in the evaluation





So how does this differ from traditional research pipeline?

Typical CS research workflow

Real world

Problem Definition

Propose Solution

Prototype

Evaluate & Refine

Code/Data

Publish

Papers

Commercialize

THE UNIVERSITY OF UTAH®

SCI www.sci.utah.edu

Translational CS research workflow

Real world

Problem Definition

Propose Solution

Prototype

Code/Data

Publish

Papers

Evaluate & Refine

Engage Community

Commercialize

THE UNIVERSITY OF UTAH®

SCI
www.sci.utah.edu

TCS Roadblocks

1. In computer science, translation is often confused with commercialization
2. Open-source techniques are often confused for translation
3. Funding agencies typically don't provide support for translation
   a) Resources to sustain and maintain research artifacts (software, data) are essential.
4. PhD programs don't allocate time and resources to translation
5. Traditional academic structures, publication venues don't value translation
6. There are a lack of exemplars


COVER FEATURE TRANSLATIONAL COMPUTING

Locale

Laboratory

Translational Research in Computer Science

David Abramson, University of Queensland
Manish Parashar, Rutgers University

There are benefits to formalizing translational computer science (TCS) to complement traditional modes of computer science research, as has been done for translational medicine. TCS has the potential to accelerate the impact of computer science research overall.

Computing and data are transforming science and society and impacting every aspect of our lives and our environment. They have become integral to the research process and have been key catalysts, complementing theory and experimentation, for recent advances and breakthroughs. Unprecedented levels of instrumentation and the exponential growth of digital data sources, coupled with pervasive computing, provide new opportunities for discovery and innovation. Examples exist in diverse application areas, from managing extreme weather events to optimizing everyday processes and improving the quality of life.

Recently, there have been dramatic changes in the nature of research-application workflows. These are driven, in part, by the greater availability and increasing scales of experimental and observational data, the ability to model phenomena more holistically, and the desire for near-real-time data processing and actuation. There have also been dramatic changes in the technology and resource landscape, complementing this change in application workflows. This includes changes in processor price and performance, the emergence of novel storage technologies, the proliferation of accelerators, the deployment of high-bandwidth/low-latency networks, and the increasing capabilities available at the network edge. In addition, through investments by research agencies worldwide, local and national cyberinfrastructure capabilities have grown in capacity and capability

Digital Object Identifier 10.1109/MC.2019.2929660
Date of publication: 27 August 2019

Translation is not commercialization

- Commercialisation almost always occurs after the research has been completed,
  - Almost never funded as part of the original research proposal
- Commercialisation implies a financial angle that has little to do with the research per-se

Use of Open Source

- Helps with distribution of a software system, but doesn't intrinsically drive impact
- No direct link between the way the software is used, and the research program. Thus, there is no explicit feedback from lessons learned in the adoption into the research itself
- More focussed on producing software that is maintained in a sustainable way, by building a distributed workforce

Funding bodies don’t typically support translation

- Evaluation criteria typically focus on the quality of the investigator team, the project quality and innovation, the feasibility and the benefit
- Translation is not usually highlighted as a desirable property; thus, a proposal might be marked down for including translational activities
- A budget that allocates resources to items such as a community trial, software distribution, software maintenance, may be pruned back to the basic research program

PhD timelines don’t support translation

- Typical PhD projects in computer science does not include translation
  - Milestones and deliverables include software prototypes, experiments and tests, producing publication outputs along with possibly software and data artefacts, and a thesis
  - Translation on its own is not consider a valid research topic
- TR adds complexity by requiring a translation phase
  - Might extend the timeline beyond that of current PhD programs

Traditional publication venues don’t value translation

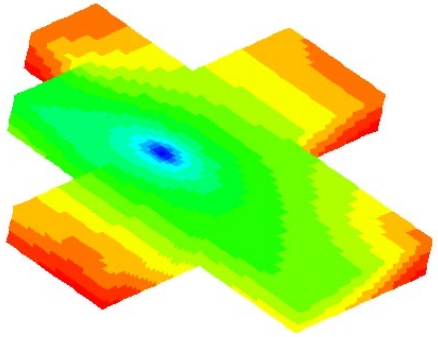
- Many editorial boards would argue translation is secondary to their scope
- More focussed on primary research outcomes in computer science
- Many translational research projects are interdisciplinary
  - Outcomes might not align well with the journal’s primary focus
- Most journals do not publish failures

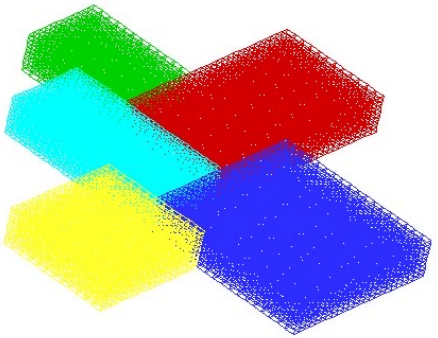
Lack of exemplars

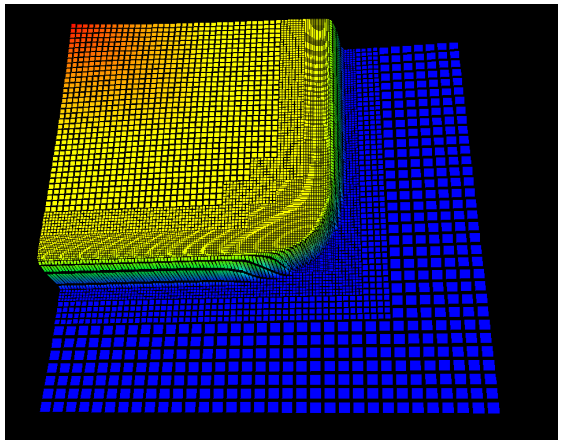
- Numerous examples of computer science research being commercialised and adopted
- Few examples of successful translational research projects
- Changing the culture in an organisation is difficult because people don't know what a good TCS project looks like

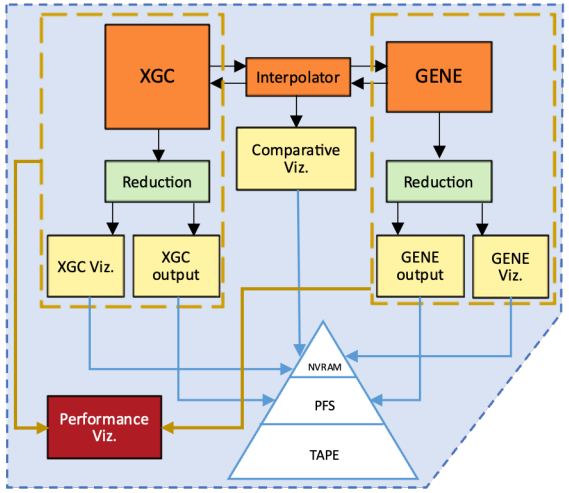
Personal Perspective: An Accidental Translationist …

- Data Management / runtime systems for large scale science
  - Dynamic, adaptive formulations
  - Coupled models and codes
  - In-situ workflows/in-transit processing
  - Integrated workflows

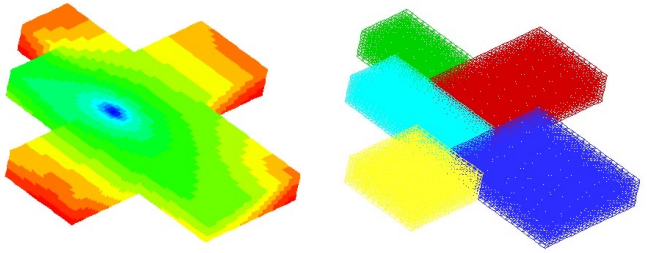




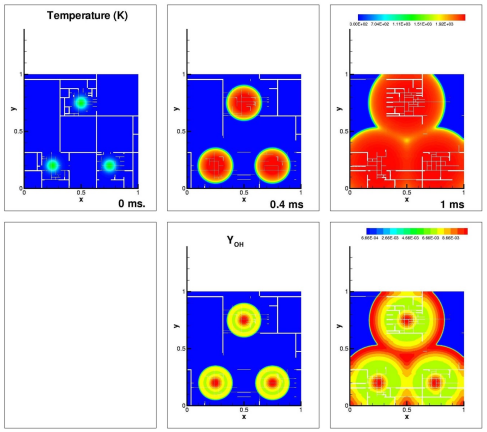




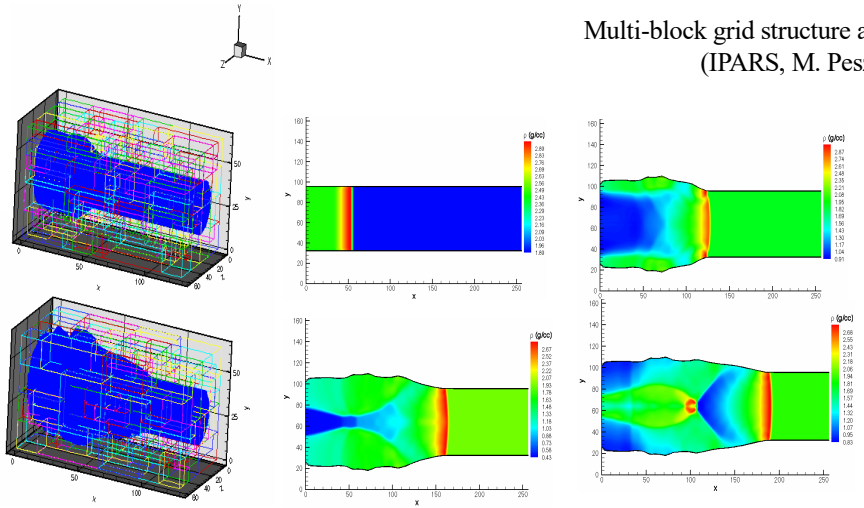
Translations Impacts



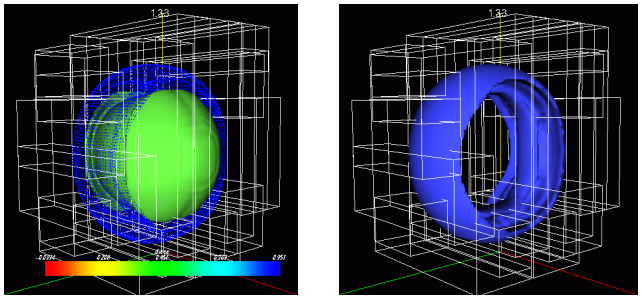
Multi-block grid structure and oil concentrations contours
(IPARS, M. Peszynska, UT Austin)



Mixture of H2 and Air in stoichiometric proportions with a non-uniform temperature fiel
(GrACE + CCA, Jaideep Ray, SNL, Livermore)



Richtmyer-Meshkov - detonation in a deforming tube - 3 levels. Z=0 plane visualized on the right (VTF + GrACE, R. Samtaney, CIT)



Blast wave in the presence of a uniform magnetic field) – 3 levels of refinement. (Zeus + GrACE + Cactus, P. Li, NCSA, UCSD)

Richtmyer Meshkov (3D)
R. Samtaney, CIT

1024x128x128, 3 levels, 2K PE's
Time: ~ 15% Memory: ~25%

THE UNIVERSITY OF UTAH®

SCI
www.sci.utah.edu

Translational Impacts

PHYSICAL REVIEW LETTERS

Highlights Recent Accepted Collections Authors Referees Search Press Abo

Stable Characteristic Evolution of Generic Three-Dimensional Single-Black-Hole Spacetimes

Featured in Physics

Boosted Three-Dimensional Black-Hole Evolutions with Singularity Excision

Gravitational Wave Extraction and Outer Boundary Conditions by Perturbative Matching

Journal of Physics: Conference Series

OPEN ACCESS

Toward a first-principles integrated simulation of tokamak edge plasmas

Journal of COMPUTATIONAL CHEMISTRY

Asynchronous replica exchange for molecular simulations

Journal of Physics: Condensed Matter

PAPER

Nucleosome positioning and composition modulate *in silico* chromatin flexibility

SC97 · Technical Paper

TOC Authors Sessions Abstracts PostScript

A Common Data Management Infrastructure for Adaptive Algorithms for PDE Solutions

THE UNIVERSITY OF UTAH®

Towards Dynamic Data-Driven Management of the Ruby Gulch Waste Repository

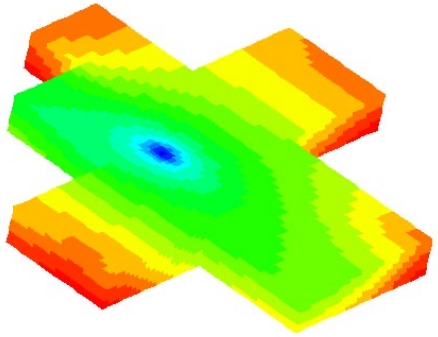
SPE 37979

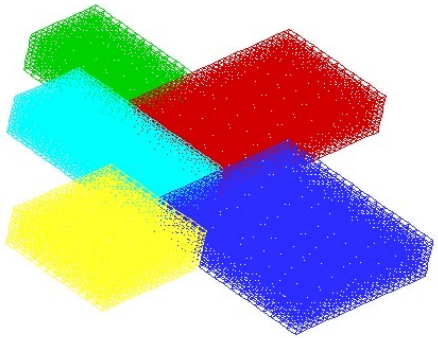
A New Generation EOS Compositional Reservoir Simulator: Part I – Formulation and Discretization.

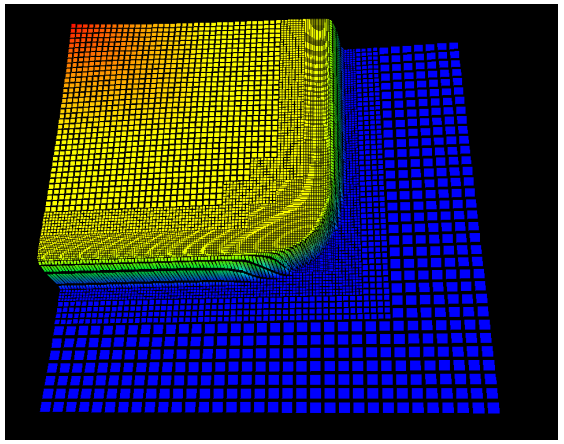
Variable Resolution Topographic Mapping of Ancient Fluvial Landscapes in Australia

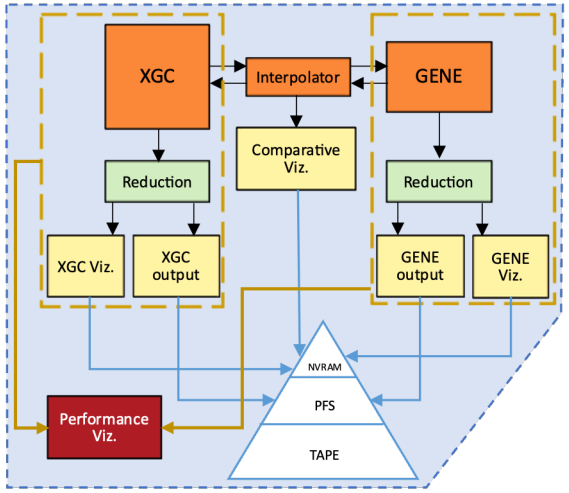
Personal Perspective: An Accidental Translationist …

- Data Management / runtime systems for large scale science
  - Dynamic, adaptive formulations
  - Coupled models and codes
  - In-situ workflows/in-transit processing
  - Integrated workflows
- Lost in translation …
  - Translation not part of the research plan
  - Lack of funding/support for translation
  - Academic career-path required reprioritization
  - But many lessons learnt that informed subsequent work









Conclusion

- CS research, innovations are transforming science and society
- TCS complements traditional CS research models (foundational, use-inspired, applied) and can accelerate and amplify the impact of computer science research
- There are benefits to formalizing TCS to complement traditional modes of computer science research
  - Several issues: Funding models, reward structures, publication venues, education and training, etc.

Call for Papers:

IEEE CiSE Department: Case Studies in Translational Computer Science

Editors:

Manish Parashar, Scientific Computing and Imaging Institute, University of Utah

David Abramson, Centre for Research Computing, The University of Queensland

Description: Our new CISE department explores how findings in fundamental research in computer, computational, and data science translate to technologies, solutions, or practice for the benefit of science and engineering, and society. Specifically, each department article will highlight impactful translational research examples in which research has successfully moved from the laboratory to the field and to the community. The goal is improving understanding of underlying approaches, exploring challenges and lessons learned, with the overarching aim to formulate translational research processes that are broadly applicable.

THE UNIVERSITY OF UTAH®

SCI
www.sci.utah.edu

Thank you!

THE UNIVERSITY OF UTAH®

SCI
www.sci.utah.edu