Translational Computer Science as a Paradigm Underpinning eScience

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Introduction

- Translational Research
  - Medicine
  - Computer Science
- Exemplars
  - Nimrod
  - Guard
  - Others …
- Important issues for TCS
- Laboratory Scale Matters
- The role of students
- What could be done locally

In memory of Ken Kennedy

… the theoretical impact of this work was matched by a tremendous practical impact, as Kennedy's work has had a profound influence in the commercialization of automatic vectorizing and parallelizing compilers.
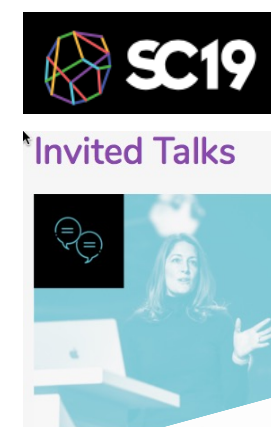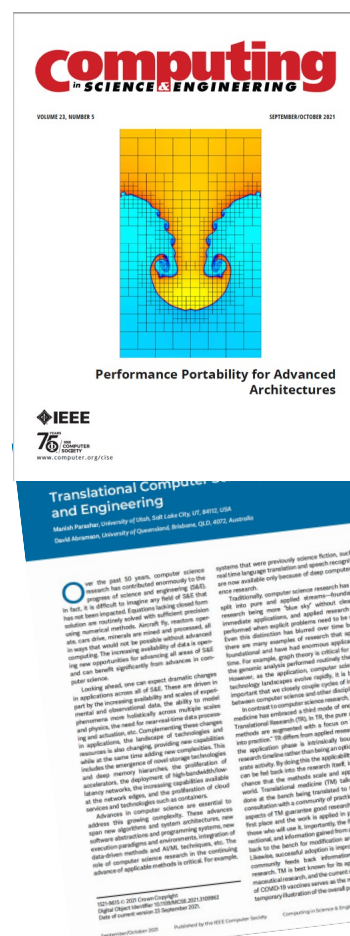
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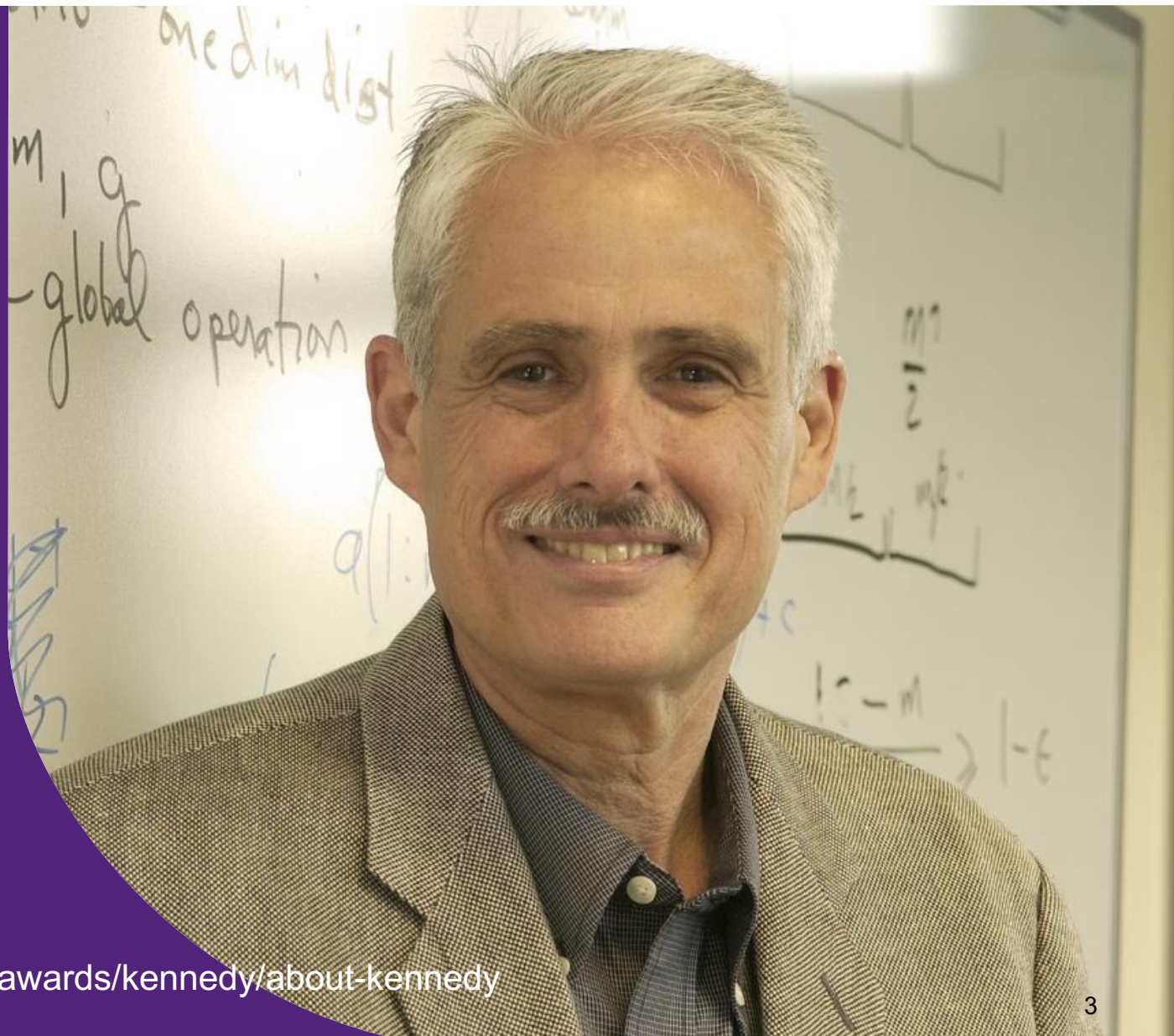
The role of a French chateaux and red wine …
with Manish Parashar

Workshop on CCDSC, Lyon France
Jack Dongarra, Bernard Tourancheau

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Background: Translational Medicine

- An "interdisciplinary branch of the biomedical field supported by three main pillars:
  - Benchside, Bedside and Community.
  - Combine 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 (driver).
  - 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

- In TM, translation relies on
  - Taking research from the laboratory Bench to the Bedside
  - More recent refinements involve Community
    - healthy populations, patients and medical practitioners.
- In TCS, translation relies on
  - Taking research from the laboratory Laboratory to the 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

Translational Computer Science

- Research that bridges
  - foundational,
  - use-inspired
  - applied research
    - with the delivery and deployment of its outcomes to a target community.
- Research that supports essential bi-direction interplays where delivery and deployment processes inform the research.

Accidental Translationists

- Joint work between CSIRO and EPAv
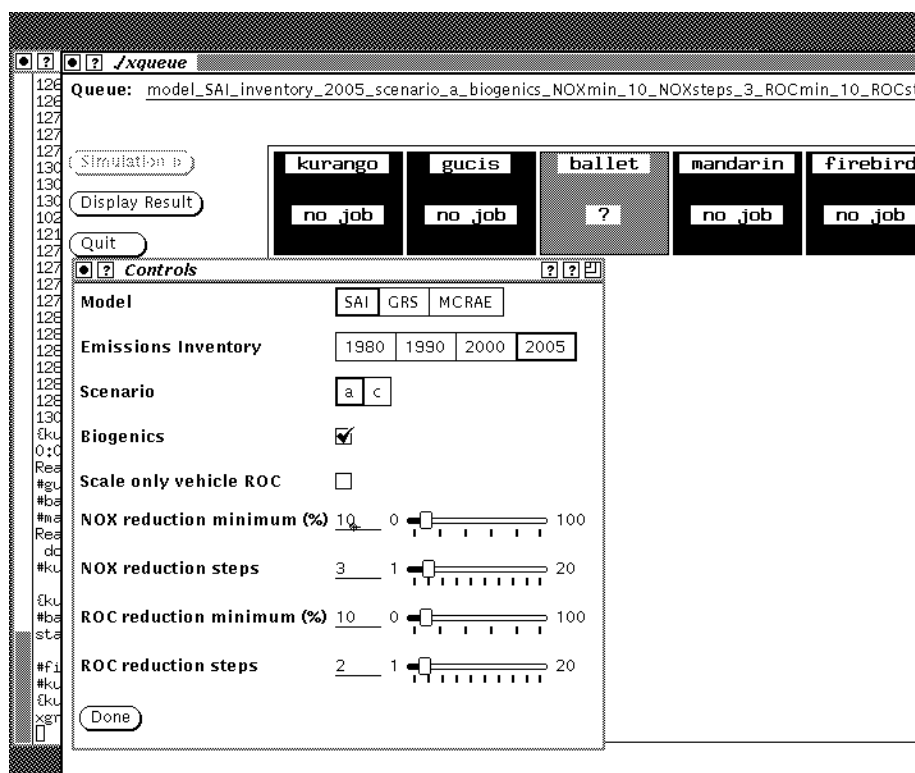
Modelling Photochemical Pollution using Parallel and Distributed Computing Platforms

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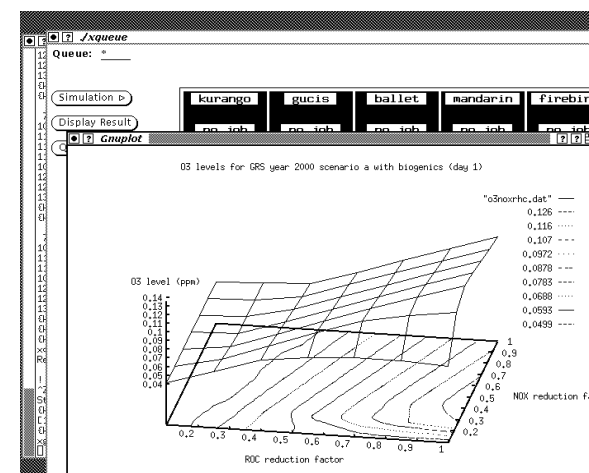Royal Melbourne Institute of Technology
P. O. Box 2476V,
Melbourne, 3001

Proceedings of PARLE-94, pp 478 - 489, Athens, Greece, July 1994

Accidental Translationists …

- The term Translational Medicine didn't come into widespread use until the mid 2000s
- The model for translational computer science presented was born from our experiences but we had no road map to follow.
- The projects were arguably successful in performing some degree of translation, but the path was difficult.
- In formalising the model and addressing the roadblocks, we believe that a translational research process in computing should be better defined and supported.
- Once the choice is made that a piece of research is to be translational, the steps to achieve success should be clearer

Exemplars

A personal perspective

Nimrod supporting "real" science

- Niche distributed programming environment
    - A full parameter sweep is the cross product of all the parameters (Nimrod/G)
    - An optimization run minimizes some output metric and returns parameter combinations that do this (Nimrod/O)
    - Design of experiments limits number of combinations (Nimrod/E)
    - Workflows (Nimrod/K)
- Has survived many distributed computing platforms
    - Workstations, Clusters, Grids, Clouds
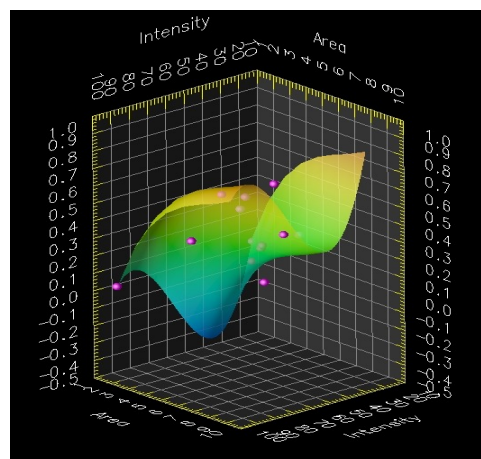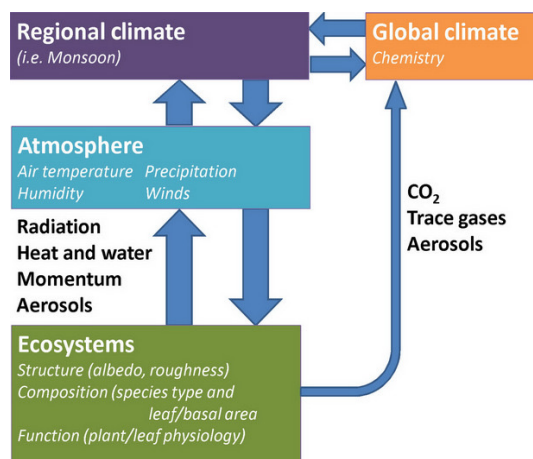- Has contributed to the understanding of HPC and distributed computing

Lenth Plot for Experiment 'Heart Cell Ca Dynamics'
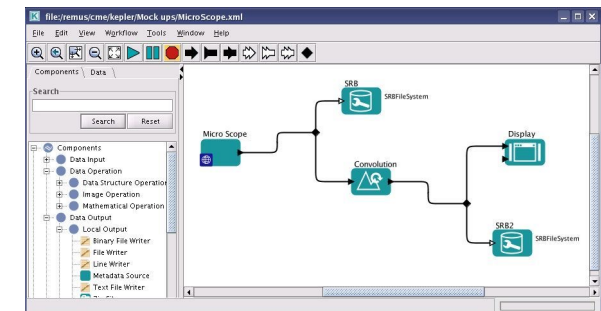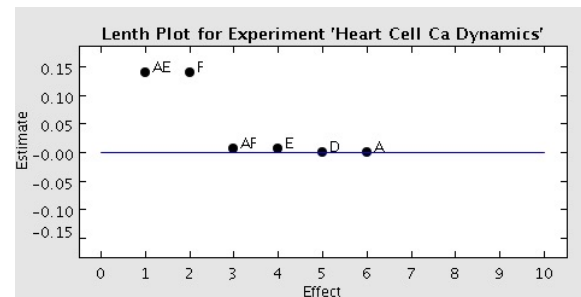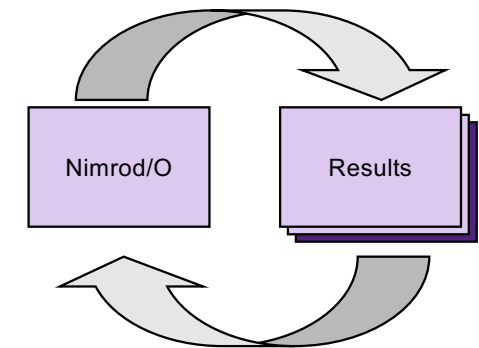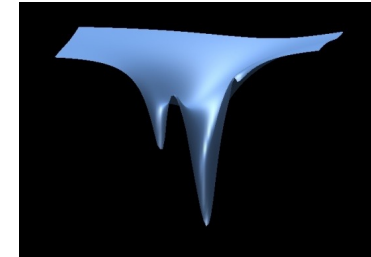
Fire in Australian savannas: from leaf to landscape
Lynch, Beringer, Uotila Monash U, AU

Science outcomes

Regional climate
(i.e. Monsoon)

Global climate
Chemistry

Atmosphere
Air temperature   Precipitation
Humidity   Winds

Radiation
Heat and water
Momentum
Aerosols

CO_2
Trace gases
Aerosols

Ecosystems
Structure (albedo, roughness)
Composition (species type and leaf/basal area)
Function (plant/leaf physiology)

Intensity   Area

RESEARCH REVIEW

Fire in Australian savannas: from leaf to landscape

JASON BERINGER[1,2], LINDSAY B. HUTLEY[3], DAVID ABRAMSON[1], STEFAN K. ARNDT[4], PETER BRIGGS[5], MILA BRISTOW[3], JOSEP G. CANADELL[5], LUCAS A. CERNUSAK[6], DEREK EAMUS[7], ANDREW C. EDWARDS[3], BRADLEY J. EVANS[8], BENEDIKT FEST[4], KLAUS GOERGEN[9,10,11], SAMANTHA P. GROVER[1,3], JORG HACKER[12], VANESSA HAVERD[5], KASTURI KANNIAH[1,13], STEPHEN J. LIVESLEY[14], AMANDA LYNCH[1,15], STEFAN MAIER[3], CAITLIN MOORE[1], MICHAEL RAUPACH[5], JEREMY RUSSELL-SMITH[3], SIMON SCHEITER[16], NIGEL J. TAPPER[1] and PETTERI UOTILA[17]

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Abstract

Savanna ecosystems comprise 22% of the global terrestrial surface and 25% of Australia (almost 1.9 million km²) and provide significant ecosystem services through carbon and water cycles and the maintenance of biodiversity. The current structure, composition and distribution of Australian savannas have coevolved with fire, yet remain driven by the dynamic constraints of their bioclimatic niche. Fire in Australian savannas influences both the biophysical and biogeochemical processes at multiple scales from leaf to landscape. Here, we present the latest emission estimates from Australian savanna biomass burning and their contribution to global greenhouse gas budgets. We then review our understanding of the impacts of fire on ecosystem function and local surface water and heat balances, which in turn influence regional climate. We show how savanna fires are coupled to the global climate through the carbon cycle and fire regimes. We present new research that climate change is likely to alter the structure and function of savannas through shifts in moisture availability and increases in atmospheric carbon dioxide, in turn altering fire regimes with further feedbacks to climate. We explore opportunities to reduce net greenhouse gas emissions from savanna ecosystems through changes in savanna fire management.

Keywords: biomass burning, climate feedbacks, greenhouse gas exchange, net ecosystem carbon balance, savanna

Introduction

Tropical savanna ecosystems account for around 22% of the global land surface (Ramankutty & Foley, 1999). Annually, up to 75% of global tropical savanna

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landscapes are burned either by natural or anthropogenic fires (Hao *et al.*, 1990) and accordingly, 50% of the total annual amount of biomass burned globally takes place in the savanna region (Hao & Liu, 1994). The wet-dry tropics of northern Australia include extensive areas of savanna vegetation, which occupy approximately 1.9 million km². This area accounts for 12% of the world's tropical savanna ecosystems, making this

CS outcomes

Fault-tolerant execution of large parameter sweep applications across multiple VOs with storage constraints

Shahaan Ayyub[*,†], David Abramson, Colin Enticott, Slavisa Garic and Jefferson Tan

Faculty of Information Technology, Monash University, Melbourne, Vic. 3145, Australia

SUMMARY

Applications that span multiple virtual organizations (VOs) are of great interest to the e-science community. However, our recent attempts to execute large-scale parameter sweep applications (PSAs) for real-world climate studies with the Nimrod/G tool have exposed problems in the areas of fault tolerance, data storage and trust management. In response, we have implemented a task-splitting approach that facilitates breaking up large PSAs into a sequence of dependent subtasks, improving fault tolerance; provides a garbage collection technique that deletes unnecessary data; and employs a trust delegation technique that facilitates flexible third party data transfers across different VOs. Copyright © 2008 John Wiley & Sons, Ltd.

1. INTRODUCTION

The computational Grid aggregates computational power and storage capacity by coupling together distributed CPU, network and storage resources [1]. The scale and nature of Grid testbeds make it possible to solve particular challenging problems in science and engineering using *parameter sweep*

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*Correspondence to: Shahaan Ayyub, Faculty of Information Technology, Monash University, Melbourne, Vic. 3145, Australia.
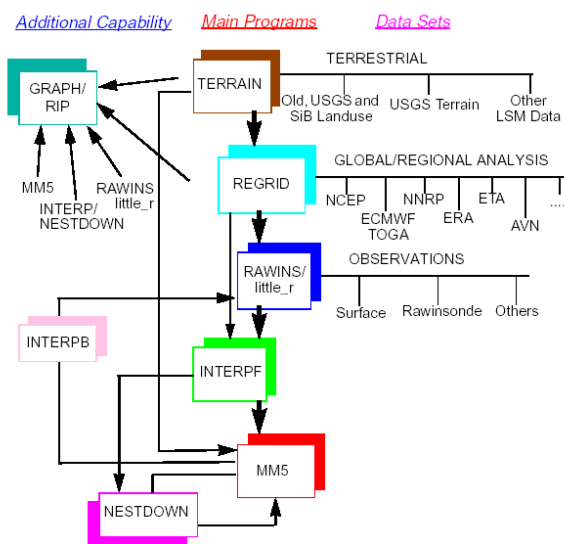†E-mail: ayyub.shahaan@infotech.monash.edu.au

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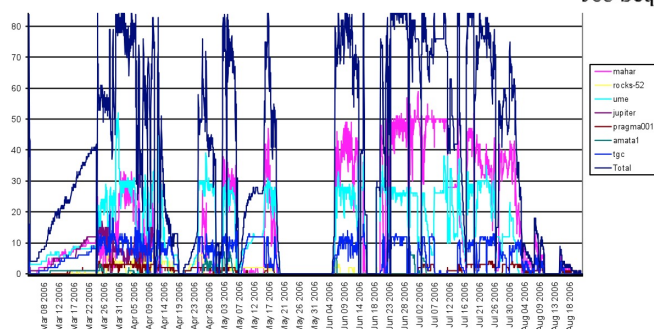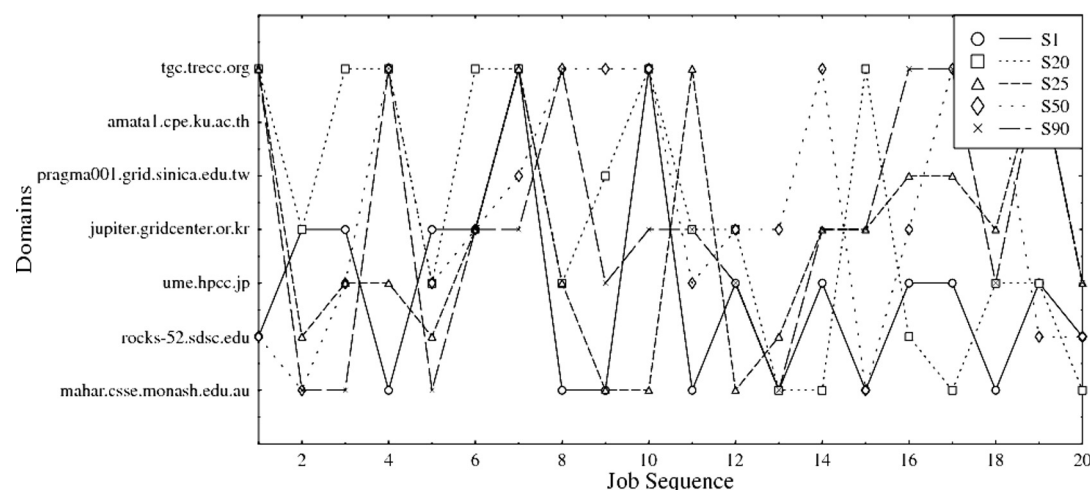
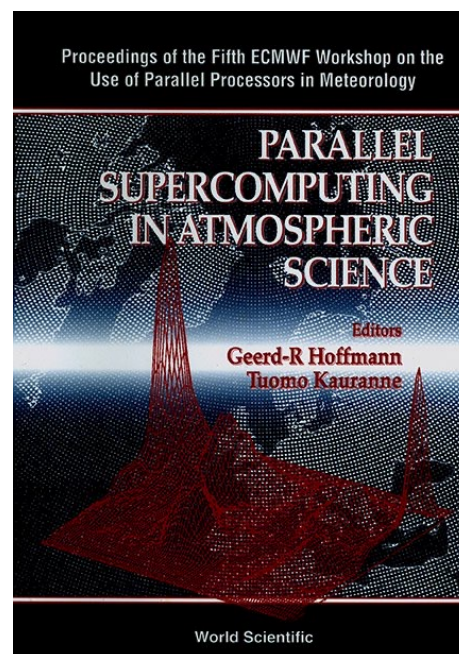# Debugging a climate model

MM5

MPMM

MPMM: A MASSIVELY PARALLEL MESOSCALE MODEL

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John Michalakes

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Argonne, Illinois 60439

1. Introduction

Static domain decomposition is a technique that provides a quick path to porting atmospheric models on distributed-memory parallel computers. However, parallel inefficiencies in the form of load imbalances and ill-tuned communication are difficult to correct without complicated and explicit re-coding. Reconfiguring the code to run on larger or smaller numbers of processors may require recompiling. Modularity and machine independence may also suffer. If full advantage is to be taken of massively parallel processing (MPP) technology, tools and techniques that allow for dynamic performance tuning and reconfiguration are required.
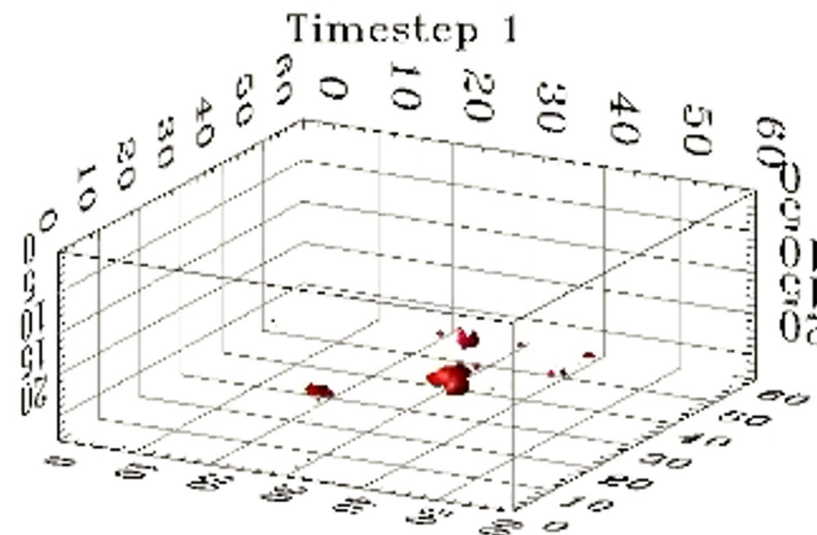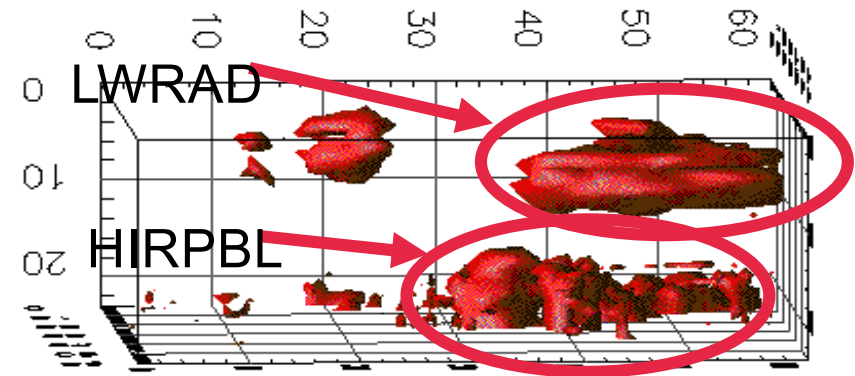
Program Composition Notation (PCN) is a language and run-time system developed at Argonne and at the California Institute of Technology for expressing parallel programs [2, 3]. It provides an intermediate layer between the application program and the physical processors of a computer. It allows the model to be statically decomposed over a *virtual* machine, but this virtual machine can be mapped and remapped dynamically over the physical computer. Programs are portable to as many machines as PCN itself, modularity is easily preserved, and communication tuning for a particular computer is encapsulated within the PCN run-time system.

In this paper we report on a project at Argonne National Laboratory to parallelize the Penn State/NCAR Mesoscale Model version 5 using a fine grain decomposition dynamically mapped and managed under PCN.

Science outcomes

- Difference in physics of planetary boundary layer

  - Computation of #steps suited to parallel execution

  - Evident in 3 dimensional visualisation

- Error in radiation time step computation

- More complete physics in long wave radiation

LWRAD

HIRPBL

Timestep 1

CS outcomes

Exemplars

Others

Pegasus Workflow Management System

Ewa Deelman - University of Southern California - PI - deelman@isi.edu

pegasus.isi.edu

Pegasus WMS

Planner

Monitoring & Provenance

Engine

HTCondor
High Throughput Computing

Scheduler

Job Queue

Submit Node

Compute Resources

Cloud Resources
Open Science Grid
HPC Systems
HTCondor Pools
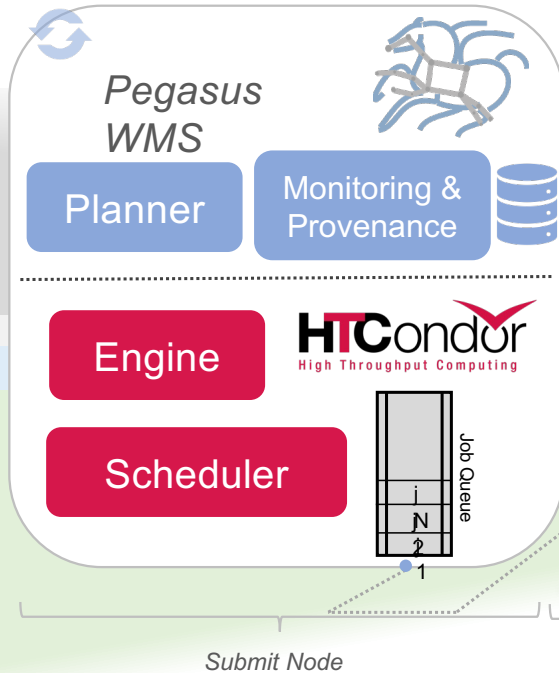
End To End Workflow Management and Execution

- Develop *portable scientific workflows* in Python, Java, and R
- Compile workflows to be *run on heterogenous resources*
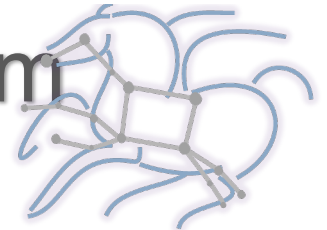- Monitor and debug workflow execution via *CLI and web-based tools*
- Recover from failures with built-in *fault tolerance mechanisms*
- *Regular release schedule* incorporating latest research and development

	2001	2003		2005		2007		2009			2011		2013			2015		2017	2018		2020
	1.0	1.1	1.2	1.3	1.4	2.0	2.1	2.2	2.3	2.4	3.0	3.1	4.0	4.1	4.2	4.3	4.4	4.5	4.6	4.7	4.8	4.9	5.0

Development: support for GT4 | task clustering | support for AWS | hierarchical workflows | pegasus-lite engine | monitoring dashboard | ensemble manager | support for containers | redesign of APIs

Research: LIGO, SCEC, and others | data cleanup algorithms | data footprint | cloud computing evaluation | MPI-based workflow engine design | Real time performance data capture | metadata capture | data integrity assurance

-0.02s

LIGO observation of colliding black holes

Campell & Borzorgnia (2008)
3s SA (g)

Hazard map indicating maximum amount of shaking at a particular geographic location generated from SCEC's CyberShake Pegasus workflow

Visualization of water on nanodiamond spheres from

Pegasus In Practice

- Laser Interferometer Gravitational Wave Observatory (LIGO) develops large scale analysis pipelines used for gravitational wave detection.
- Southern California Earthquake Center (SCEC) CyberShake project generates hazard maps using hierarchical workflows .
- Oak Ridge National Lab (ORNL) conducted studies on tRNA and nanodiamonds to improve drug delivery design principles.

NSF WIFIRE Project: 2013-2018
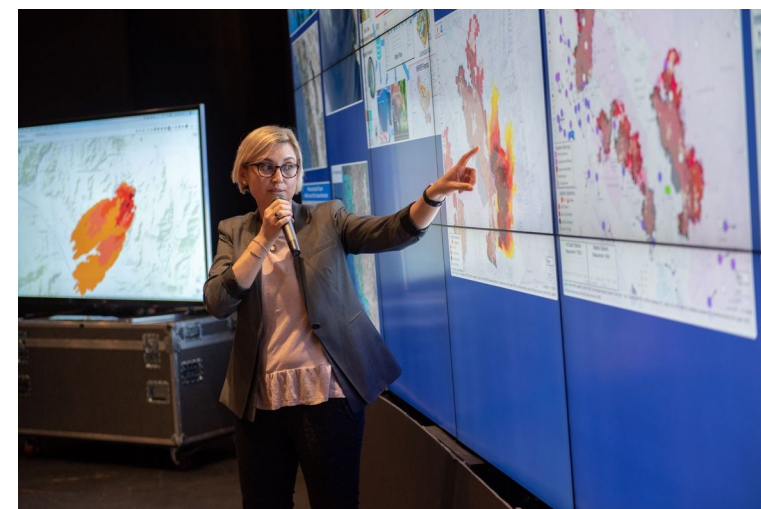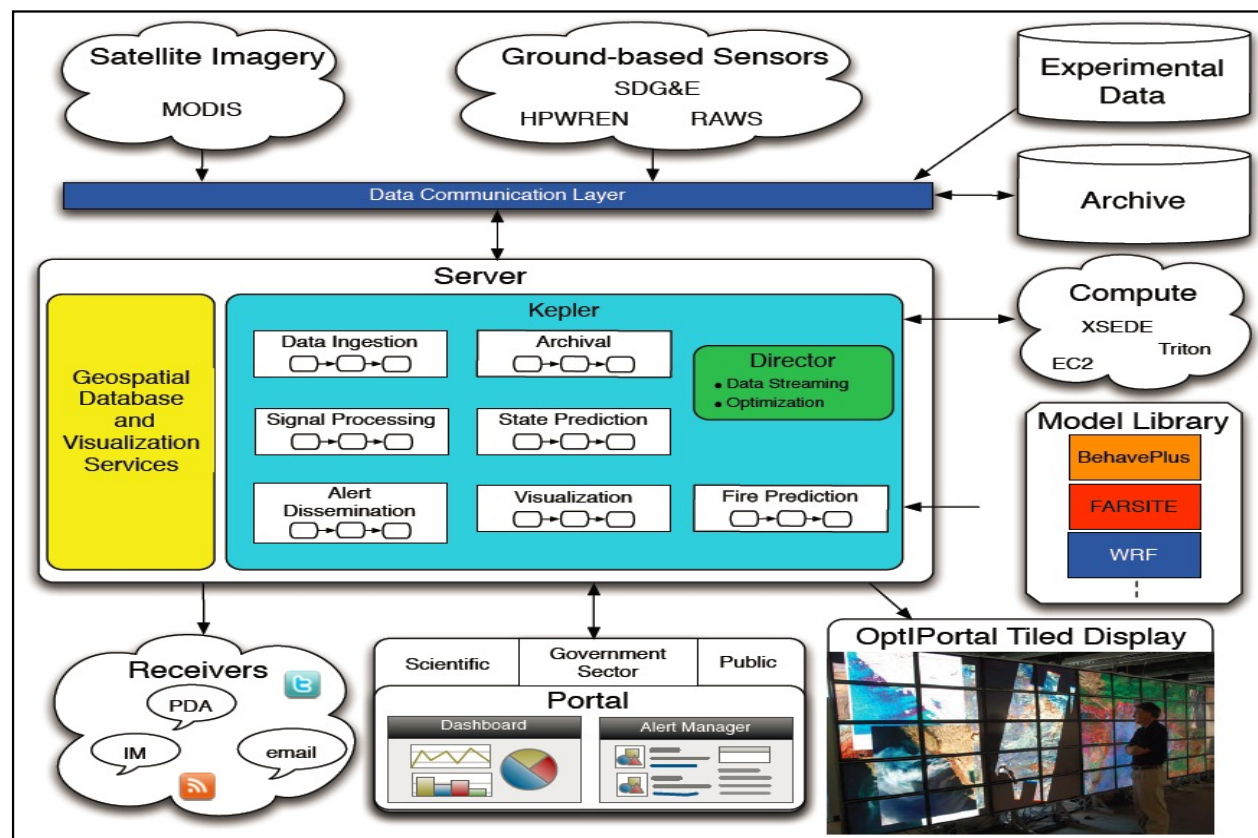
NSF-1331615

Grid Computing as Translational Research

Globus community testbed, 1998

Goal: Identify simple mechanisms to enable collaborative science in a hyper-connected world

Translational approach: Work closely with domain scientists, application developers, and resource providers on deployment, application, and evaluation of proposed mechanisms

Artifacts: Globus Toolkit (1998-2015); Globus service (2010-)

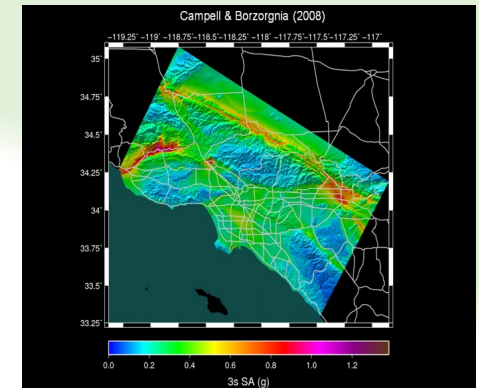**Science impact**: 10,000s of scientists worldwide via dozens of Grid deployments and application projects; 100s of science projects, including Nobel-winning physics, astronomy, climate

Computer science impact: Virtual organizations, secure and reliable remote computation, performant and reliable data sharing, workflow specification and execution

Thanks: Globus team, grid deployments, science collaborators, computer science collaborators, DOE, NSF, NASA, NIH

More info: Ian Foster (foster@anl.gov)
Carl Kesselman (carl@isi.edu)

https://doi.org/10.1016/j.jocs.2020.101214 – https://globus.org
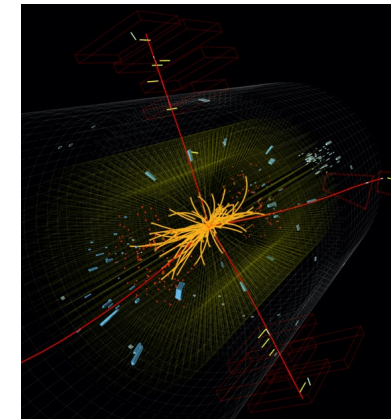
Higgs boson discovery at LHC (2012)
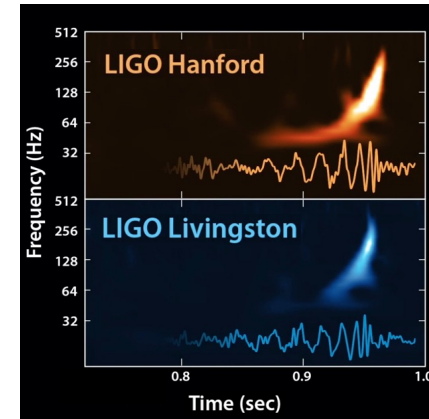
Gravitational wave detection, LIGO (2015)
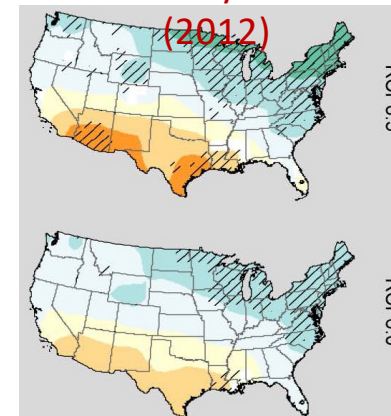
IPCC climate science: Earth System Grid
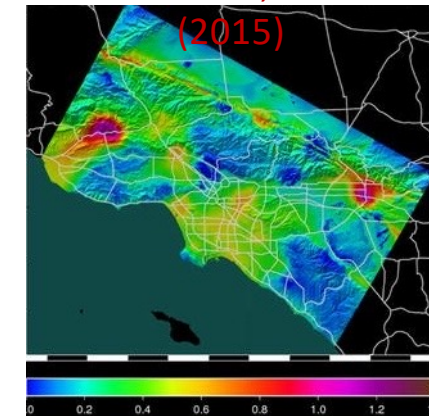
CyberShake earthquake hazard map

So how does this differ from traditional research pipeline?

Typical CS research workflow

Code

Propose
Solution

Problem
Definition

Prototype

Publish

Evaluate &
Refine

Real world

Papers

Commercialize

Translational CS research workflow

Real world

Problem Definition

Propose Solution

Prototype
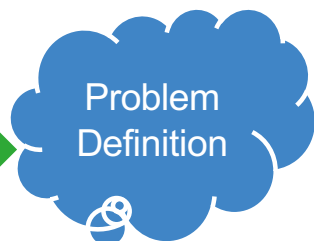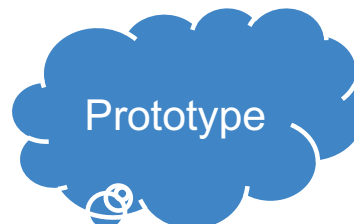
Code

Publish

Evaluate & Refine

Engage Community

Papers
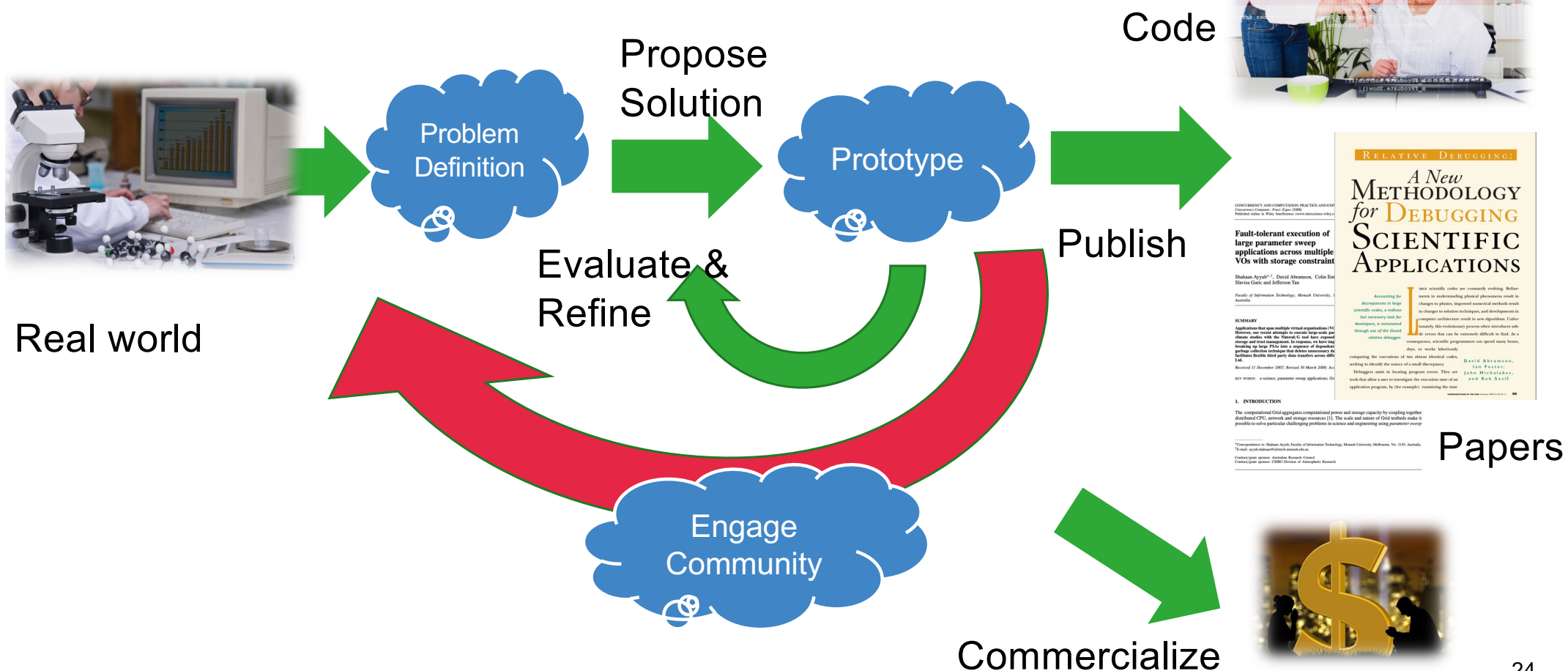
Commercialize

Roadblocks and overpasses

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

4. PhD programs don't allocate time and resources to translation

5. Traditional publication venues don't value translation

6. There are a lack of exemplars

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.

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PhD timelines don't support translation

- Typical PhD projects in computer science follow a very standard and often rigid template.
    - Students engage in a project of interest to them
    - Execute a plan much like any other research project.
    - Milestones and deliverables include software prototypes, experiments and tests, producing publication outputs along with possibly software and data artefacts.
    - At the very least, a PhD student needs to produce a thesis.
- 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.

Funding

- Currently ad hoc funding.
- Sustained funding programs and mechanisms focussed on fostering and nurturing TCS
- More money alone not solution
- Need to *build* translation into the research plan
- Funding must be used to experiment with solutions and prototypes.
- TCS typically involves substantial interaction with end users.
- Additional travel, user engagement, and provisioning of computing resources
- Translation process feeds back into the research,
  - may be a loop of research and translation rather than a linear waterfall style of workflow
- Should be free to report on both research successes, but also translation **success** or **failures**.

Venues, metrics and reward structures

- Traditional publications are not well suited to TCS.
    - Drawing on TM, new journals have been created that explicitly target translational medicine.
    - New set of similarly scoped journals and conferences.
    - Metrics, recognitions and rewards structures, especially in the academic community.
        - software and data and to track their use, citations and impact are a step in the right direction
    - Metrics that report uptake of their work, and measure how many of these have resulted in successful translation
    - Integrate metrics into promotion processes

Education and Training

- Integration of translational approaches and methodologies into more formal computer science curricula

- New materials and mechanisms for providing translational skills to practitioners, in both computer and other disciplines.
  - doctoral training centers have been established that encourage and enable trans-disciplinary research

- Extreme example, a PhD could be entirely devoted to the translation of work performed by another researcher, with no original research on the background IP per se

Laboratory Scale Matters

THE UNIVERSITY OF QUEENSLAND
AUSTRALIA

Applications

Core Technology

PRAGMA/PRIME/MURPA

UCSD

Oxford

DPI

Univ Melb

Univ Amsterdam

Univ Zurich

Pharmacy

Arts

Engineering

Information Technology

Business and Economics

Medicine

Science

Nimrod/G

Nimrod/K

Nimrod/E

Nimrod/O

Guard

Eclipse/PTP

MeSsAGE Lab

Axceleon

Guardsoft

Cray

Leica

HP

IBM

Microsoft

External Research Collaborators

Monash Research Collaborators

External Industry Collaborators

37

PRAGMA

- Strengthen Existing and Establish New Collaborations

- Work with Science Teams to Advance Grid Technologies and Improve the Underlying Infrastructure

- In the Pacific Rim and Globally

Resource Name	Number of Nodes	CPU speed
rocks-52.sdsc.edu	60	2.4
tgc.trecc.org	12	2.0
pragma001.grid.sinica.edu.tw	4	2.4
amata1.cpe.ku.ac.th	14	1.4
jupiter.gridcenter.org.kr	16	1.4
ume.hpcc.jp	64	1.4
mahar.infotech.monash.edu.au	50	3.0
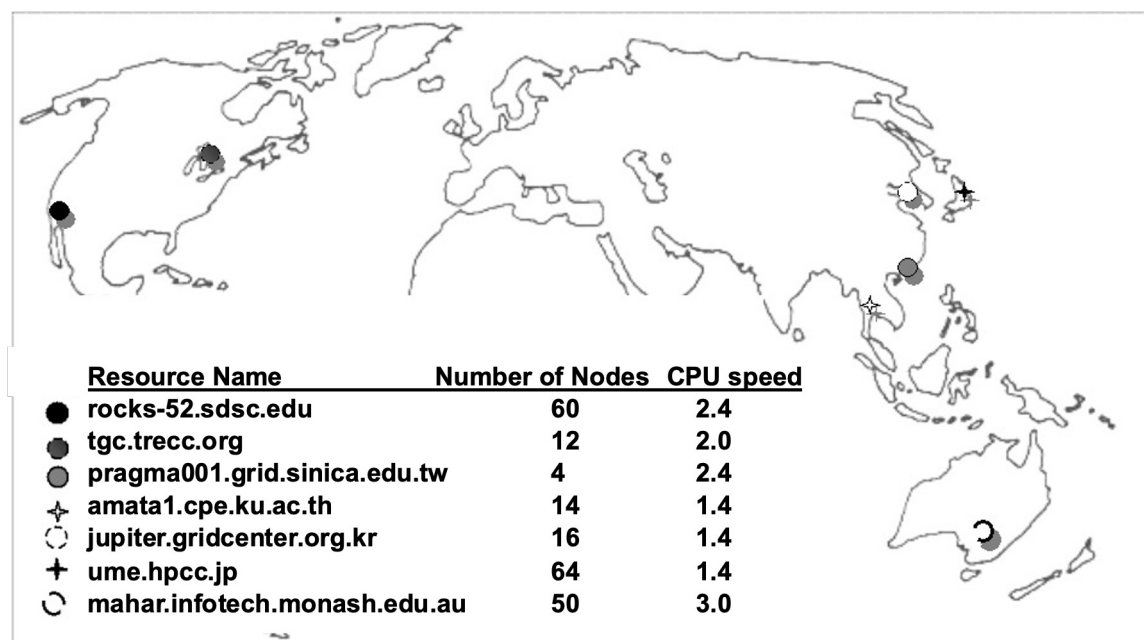
Leveraging the PRAGMA testbed: Technical

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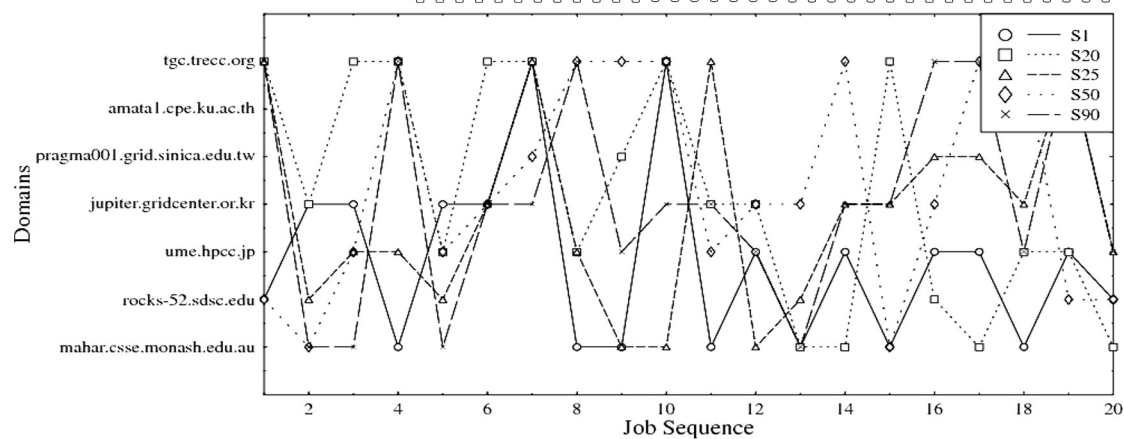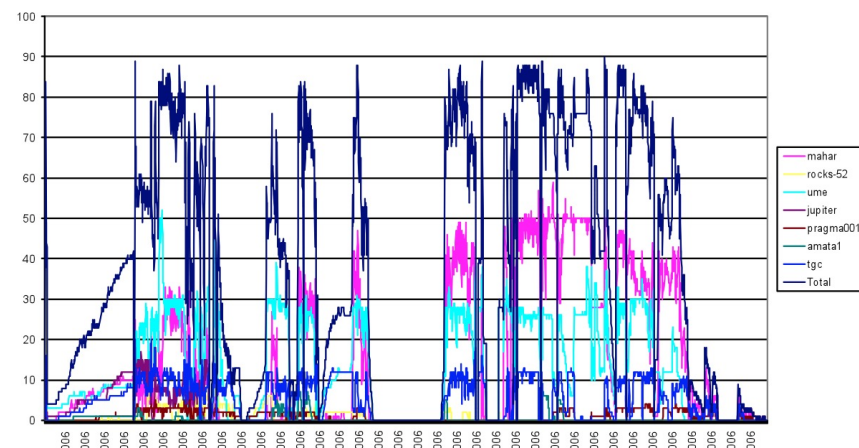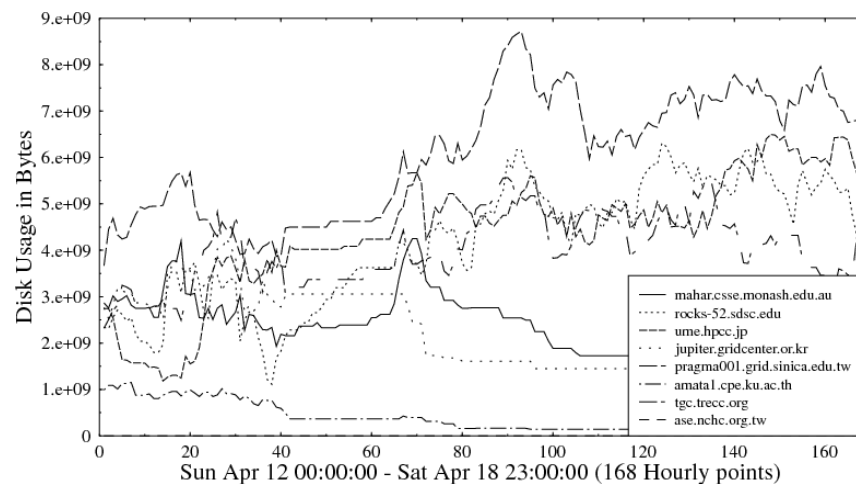
Leveraging the PRAGMA testbed: Social

Research Apprenticeship Joint Mentors @ Home & Host site			
Define Project	Prepares for Project	Executes Project	Presents Outcomes

Undergraduate Students

Pre-departure Training	Weekly Questions	Post-return debrief	Career Advice
Cultural Competencey			Professional

Before Departure — During internship — After Return

Research Experience

Collaborations

Publications

Software

Host-site researchers

Cultural Awareness

Globally Aware Workforce

Outputs & Outcomes

A typical PRIME project
Lead placement for CRT
Revelli, Kirchoffs, McCulloch UCSD

- Study left bundle branch block
- Determine the optimal pacing sites for CRT
- 2 or 3 leads are inserted into the heart
- Challenges:
  - Placing the leads
  - Scar tissue effects pacing
- Continuity and Nimrod to explore different pacing sites

MURPA/QURPA annual seminar stream

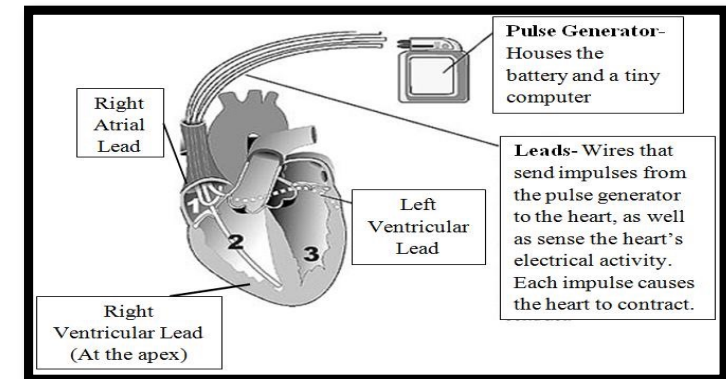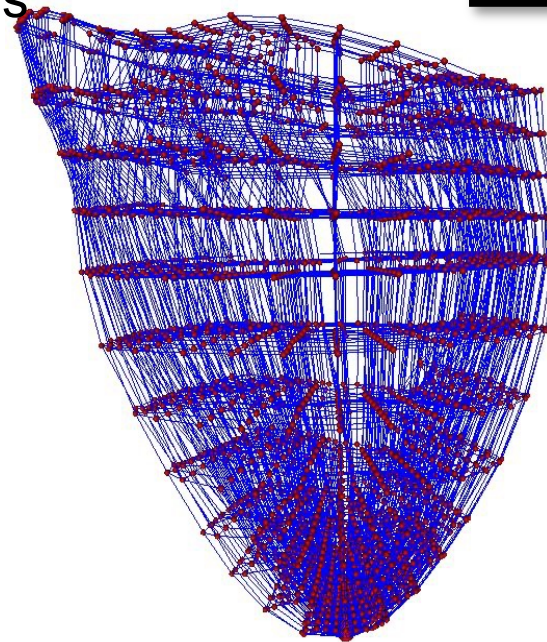|	
Nancy Wilkins-Diehr	Science Gateways and their tremendous potential for Science a
Jurgen Schulze	Latest Developments in Virtual Reality at Calit2
Ania Sher	Mathematical models of cardiac muscle cells: Predicting drug-in
Robert Konecny	Multiscale Modeling of Proteins
Phil Papadopolous	Extending Rocks Clusters into Amazon EC2 Using Condor
Wilfred Li	Workflows for Computer Aided Drug Discovery: New Twitter for
Philip Bourne	New Modes of Scholarly Communication
Mike Norman	Gordon: A New Kind of Supercomputer for Data-Intensive Appl
Larry Smarr	Global Climatic Disruption and its Impact on Victoria and California
Sameer Tilak	Cyberinfrastructure for Large-Scale Environmental Observing Systems
Bill Gropp	Enabling the Next Generation of Scalable Systems
Dr. Edee Wiziecki	Using Virtual Machines to accommodate Computational Chemistry in courses and classrooms
Alan Craig	Augmented Reality
Dr. Robert A. Fiedler	Applications on the Blue Waters Sustained Petascale System
Dr. Radha Nandkumar	Global connections with Child Health Informatics
Dr. Brett Bode	Software Development in Petascale Computing
Dr. Steven Gottlieb	Lattice QCD: Challenges of Scaling to Peta and Exaflop Speeds

What could be done locally?

- Multi-disciplinary R&D is essential
  - Build supportive structures
- Funding agencies typically don't provide support for translation
  - Provide out of band support for translation
  - Build cross university mechanisms for translation
  - Provide resources to sustain and maintain research artifacts (software, data)
- PhD programs don't allocate time and resources to translation
  - Provide time extentions for translation
  - Tweak PhD criteria
- Traditional publication venues don't value translation
  - Academic promotion criteria don't value translation
    - Alter focus on traditional metrics
  - Translationists don't comfortably into existing career profiles
    - Third career track for supporters
- Laboratory scale matters
  - Build and support larger laboratories
    - Heterogenous support
    - Multi-disciplinary foci

There's often a back story …

It's 1990 and the World Wide Web is making its way into homes all across the world. Everyone wants in on the action, including Charles — a PhD student with an impressive list of citations and a Herculean ego, but not much else. How far will he go to make a name for himself and how many people will he squash to get there?

"I think the Internet's going to revolutionize life," said Charles
"Mmm. How so?" uttered Holywell
"I don't know." Charles began jiggling his right leg, coins rattling in his pocket. "I just get the impression it's going to make a big difference."

"We've all known a Charles. Abramson's wry story of an academic's cynical ambition could easily play out in any university, business or government"
Peter Greste, Journalist and Author of 'The First Casualty.'

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Thank you and Questions