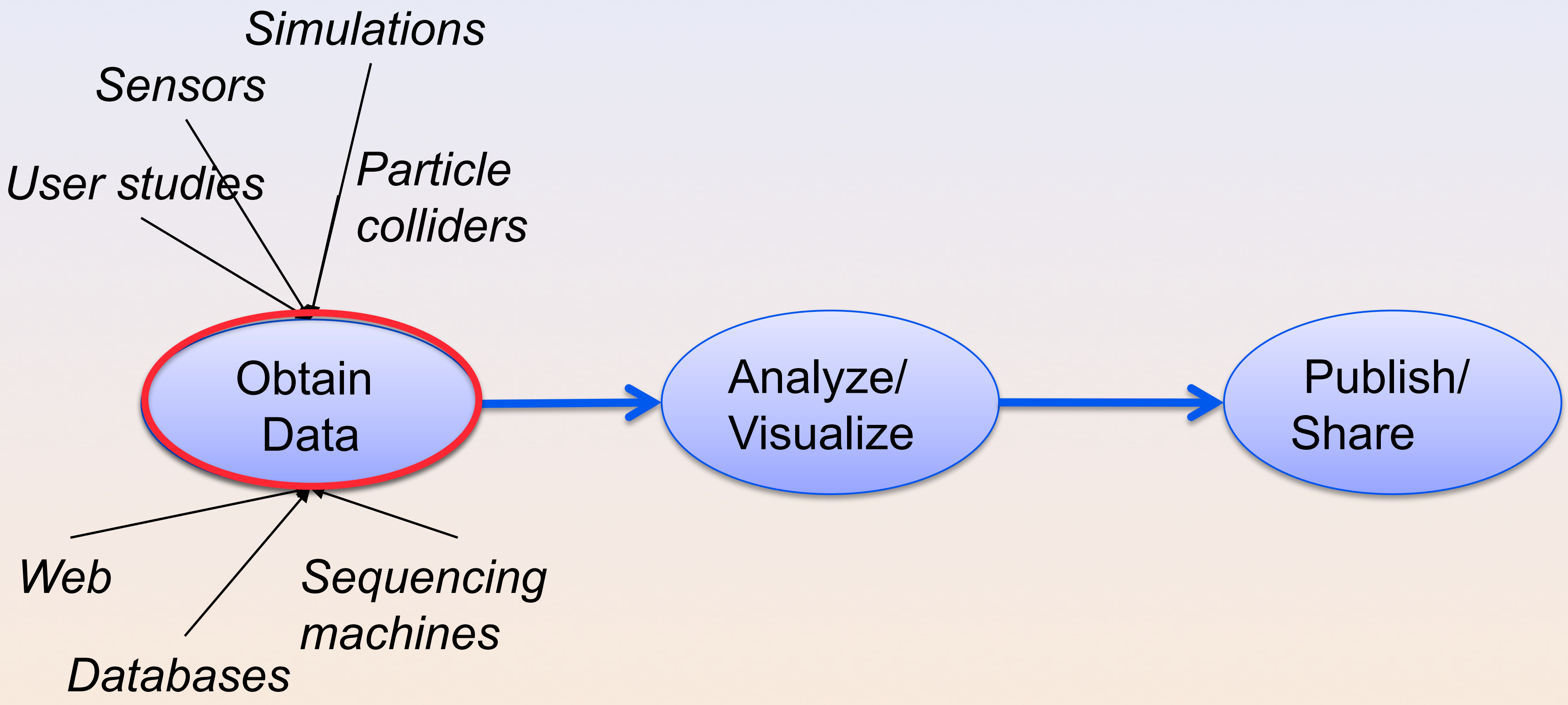
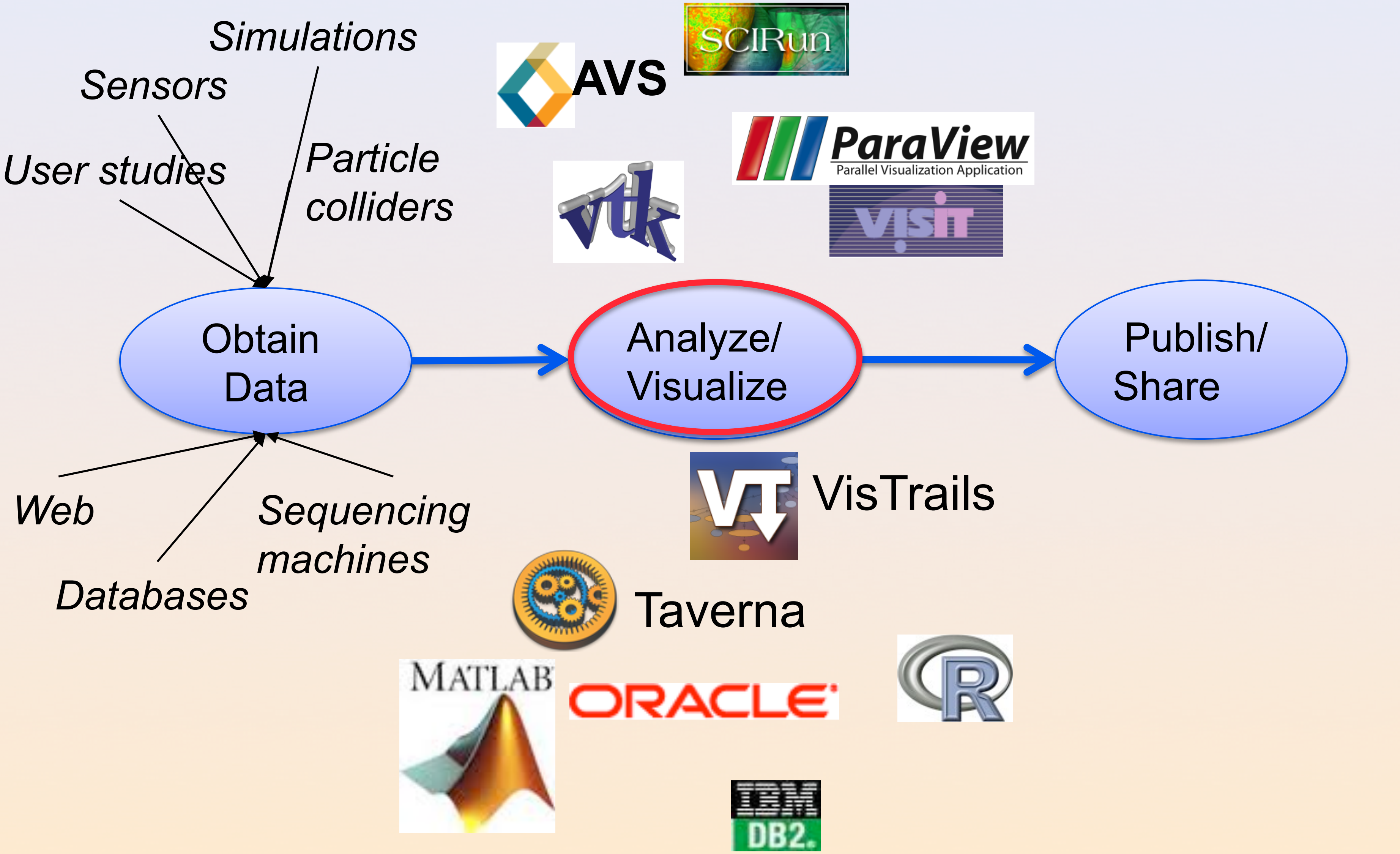
Publishing Reproducible Results with VisTrails

Juliana Freire and Claudio Silva
VisTrails Group
Scientific Computing and Imaging Institute
School of Computing
University of Utah

Science Today: Data Intensive



Science Today: Data + Computing Intensive



Simulations

Sensors

User studies

Particle colliders

Obtain Data

Analyze/ Visualize

Publish/ Share

Web

Databases

Sequencing machines

AVS

SCIRun

ParaView Parallel Visualization Application

vtk

VisIt

VisTrails

Taverna

MATLAB

ORACLE

R

IBM DB2.

Science Today: Data + Computing Intensive

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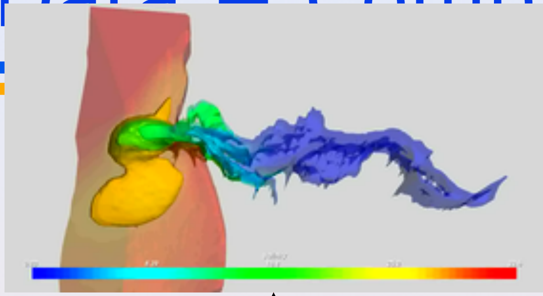

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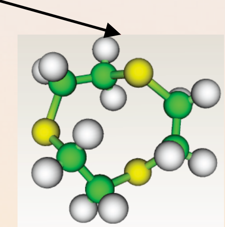
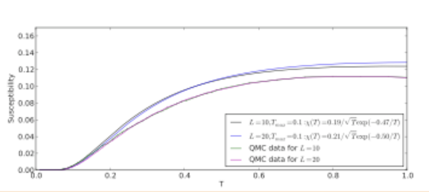
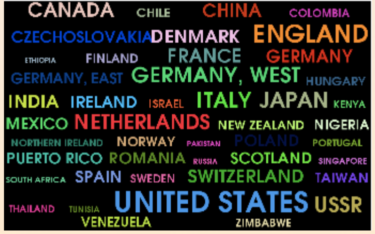
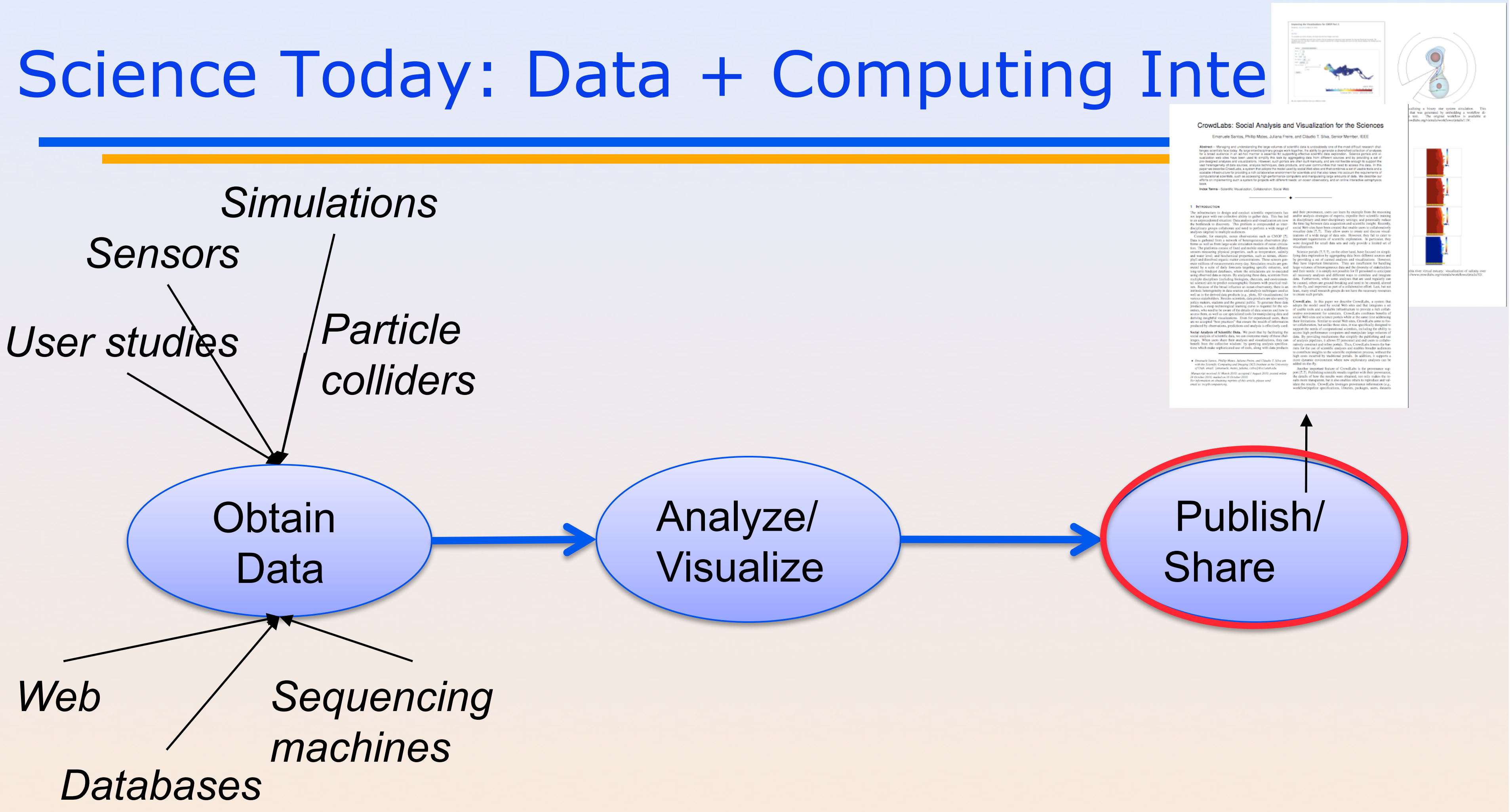



Susceptibility
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
0.0
0.2
0.4
0.6
0.8
1.0
T
$L=10, T_{max}=0.1 : \chi(T)=0.19/\sqrt{T}\exp(-0.47/T)$
$L=20, T_{max}=0.1 : \chi(T)=0.21/\sqrt{T}\exp(-0.50/T)$
QMC data for $L=10$
QMC data for $L=20$


CANADA CHILE CHINA COLOMBIA
CZECHOSLOVAKIA DENMARK ENGLAND
ETHIOPIA FINLAND FRANCE GERMANY
GERMANY, EAST GERMANY, WEST HUNGARY
INDIA IRELAND ISRAEL ITALY JAPAN KENYA
MEXICO NETHERLANDS NEW ZEALAND NIGERIA
NORTHERN IRELAND NORWAY PAKISTAN POLAND PORTUGAL
PUERTO RICO ROMANIA RUSSIA SCOTLAND SINGAPORE
SOUTH AFRICA SPAIN SWEDEN SWITZERLAND TAIWAN
THAILAND TUNISIA UNITED STATES USSR
VENEZUELA ZIMBABWE

Science Today: Data + Computing Inte



CrowdLabs: Social Analysis and Visualization for the Sciences

Emanuele Santos, Phillip Mates, Juliana Freire, and Cláudio T. Silva, Senior Member, IEEE

Abstract— Managing and understanding the large volumes of scientific data is undoubtedly one of the most difficult research challenges scientists face today. As large interdisciplinary groups work together, the ability to generate a diversified collection of analyses for a broad audience in an ad-hoc manner is essential for supporting effective scientific data exploration. Science portals and visualization web sites have been used to simplify this task by aggregating data from different sources and by providing a set of pre-designed analyses and visualizations. However, such portals are often built manually, and are not flexible enough to support the vast heterogeneity of data sources, analysis techniques, data products, and user communities that need to access this data. In this paper we describe CrowdLabs, a system that adopts the model used by social Web sites and that combines a set of usable tools and a scalable infrastructure for providing a rich collaborative environment for scientists and that also takes into account the requirements of computational scientists, such as accessing high-performance computers and manipulating large amounts of data. We describe our efforts on implementing such a system for projects with different needs: an ocean observatory, and an online interactive astrophysics book.

Index Terms—Scientific Visualization, Collaboration, Social Web

1 Introduction

Science Today: Incomplete Publications

- Publications are just the tip of the iceberg
  - Scientific record is incomplete--- to large to fit in a paper
  - Large volumes of data
  - Complex processes
- Can’t (easily) reproduce results

CrowdLabs: Social Analysis and Visualization for the Sciences

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Index Terms—Scientific Visualization, Collaboration, Social Web

Microsoft® PowerPoint®
ORACLE
VT
IBM DB2.
MATLAB
R
vtk
CANADA CHINA DENMARK ENGLAND FRANCE GERMANY WEST INDIA ITALY JAPAN MEXICO NETHERLANDS NORWAY PUERTO RICO ROMANIA SCOTLAND SPAIN SWITZERLAND UNITED STATES USSR

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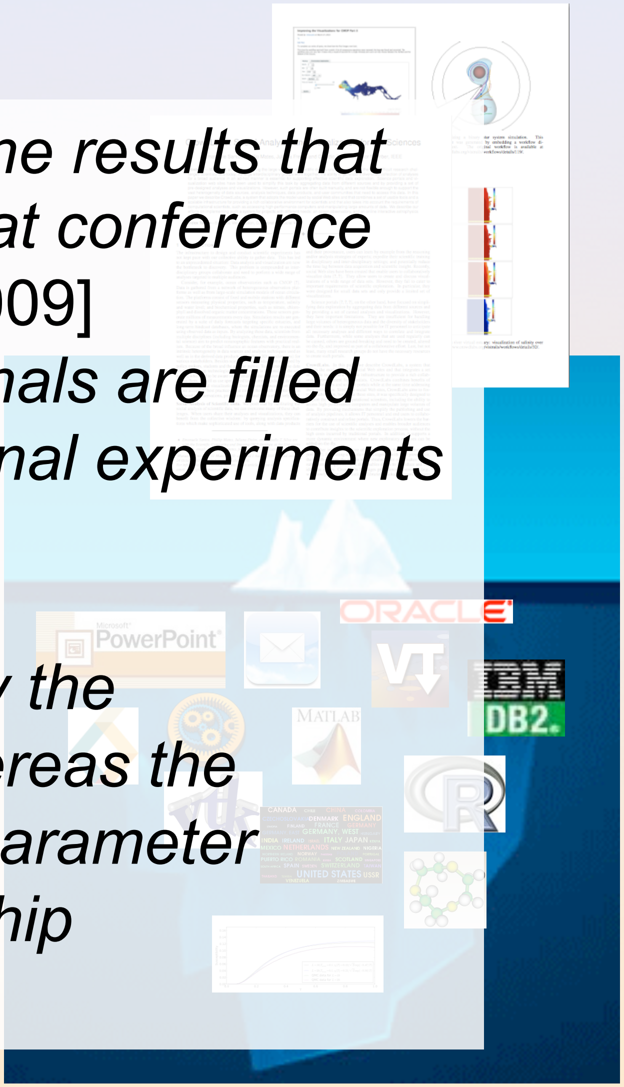
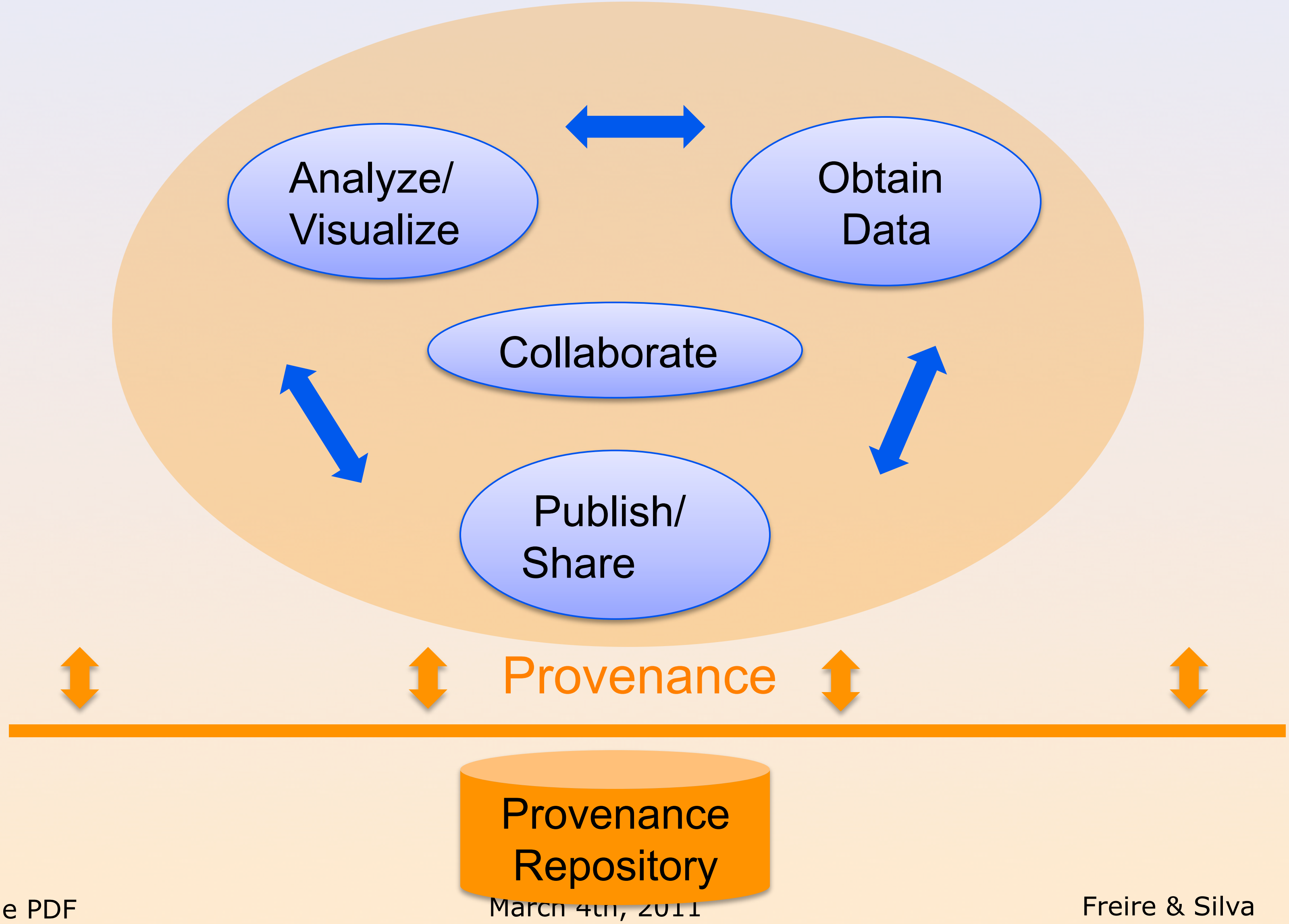


"It's impossible to verify most of the results that computational scientists present at conference and in papers." [Donoho et al., 2009]

"Scientific and mathematical journals are filled with pretty pictures of computational experiments that the reader has no hope of repeating." [LeVeque, 2009]

"Published documents are merely the advertisement of scholarship whereas the computer programs, input data, parameter values, etc. embody the scholarship itself." [Schwab et al., 2007]

Need Provenance-Rich Science



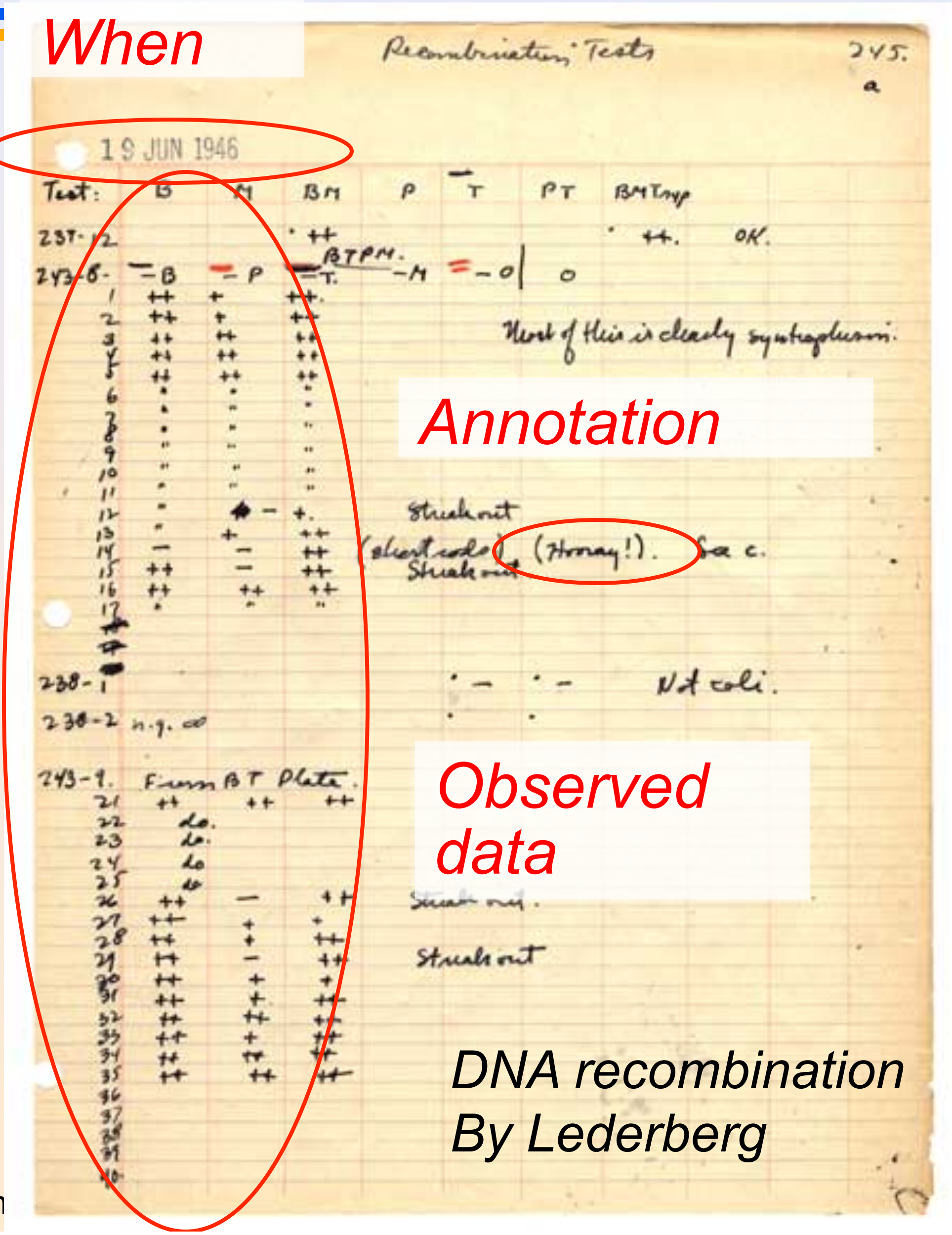
Provenance in Science

- Interpret and *reproduce* results
- Understand the experiment and chain of reasoning that was used in the production of a result
- Verify that an experiment was performed according to acceptable procedures
- Identify the inputs to an experiment were and where they came from
- Assess *data quality*
- Track *who* performed an experiment and who is responsible for its results

Provenance is as (or more!) important as the results

Provenance in Science

- Not a new issue!
- Lab notebooks have been used for a long time
- What is new?
  - Large volumes of data
  - Complex analyses—computational processes
- Writing notes is no longer an option
- Need infrastructure to capture and manage provenance information



Recombination Tests 245. a

19 JUN 1946

Test: B M BM P T PT BMTmp

Most of this is clearly cytoplasmic.

Struck out

(Hooray!)

Not coli.

From BT Plate.

When

Annotation

Observed data

DNA recombination
By Lederberg

Provenance-Rich Publications

- Bridge the gap between the scientific process and publications
  - The scientific record needs to be *complete and trustworthy*
  - Papers with *deep* captions

- Show me the proof: results that can be reproduced and validated
  - Encouraged by ACM SIGMOD, a number of journals, funding agencies, academic institutions (e.g., http://www.vpf.ethz.ch/services/researchethics/Broschure)

Provenance-Rich Publications: Benefits

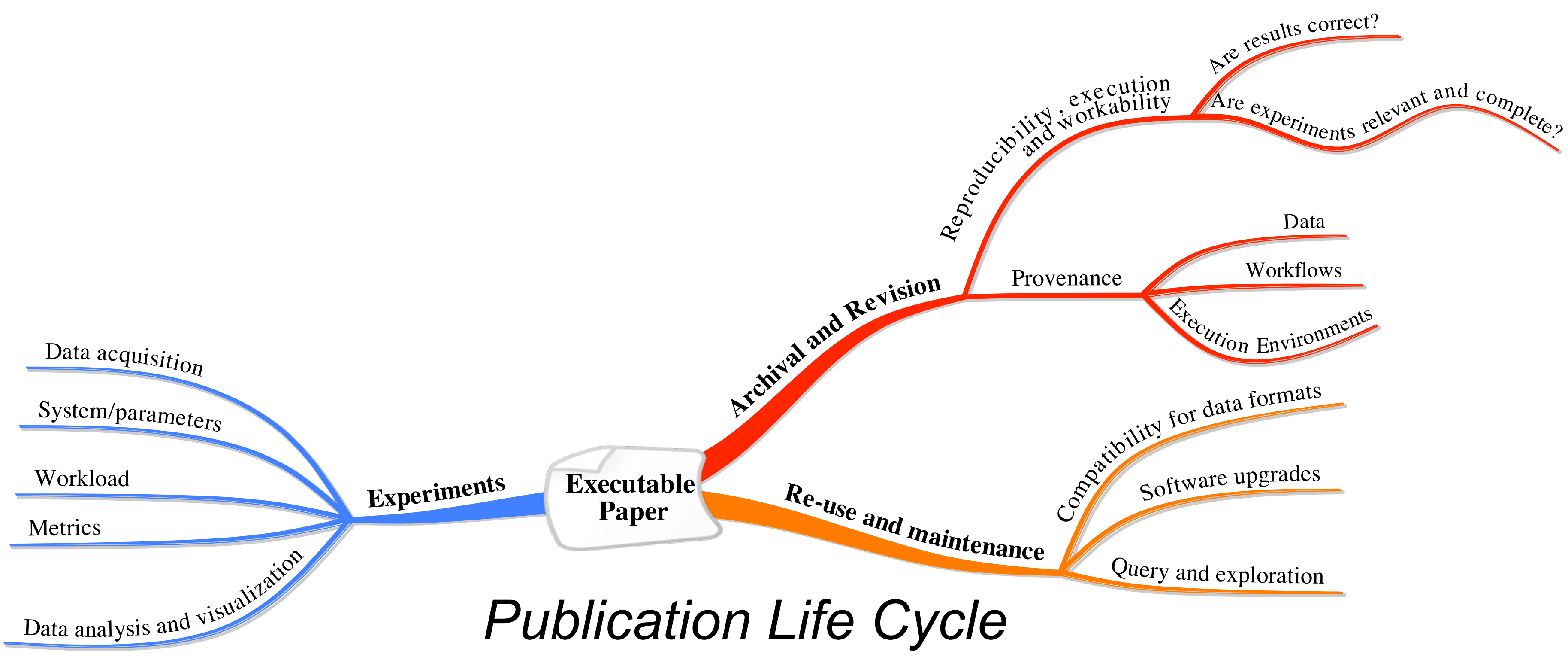
- Produce more knowledge---not just text
- Allow scientists to stand on the shoulders of giants (and their own…)
  - Science can move faster!
- Higher-quality publications
  - Authors will be more careful
  - Many eyes to check results
- Describe more of the discovery process: people only describe successes, can we learn from mistakes?
- Expose users to different techniques and tools: expedite their training; and potentially reduce their time to insight

Provenance-Rich Publications: Challenges

- It is too hard, time-consuming for authors to prepare compendia of reproducible results
  - Data, computations, parameter settings, etc.
- It is too hard for reviewers (and readers) to install, compile, and reproduce experiments
  - Different OSes, library versions, hardware, large data, incompatible data formats…
- Our goal: simplify the process of sharing, reviewing and re-using scientific experiments and results

Our Approach

- Focus on computational experiments: Reproduce, validate and re-use
- *Integrate* data acquisition, derivation, analysis, visualization, and their *provenance* with the publication life cycle

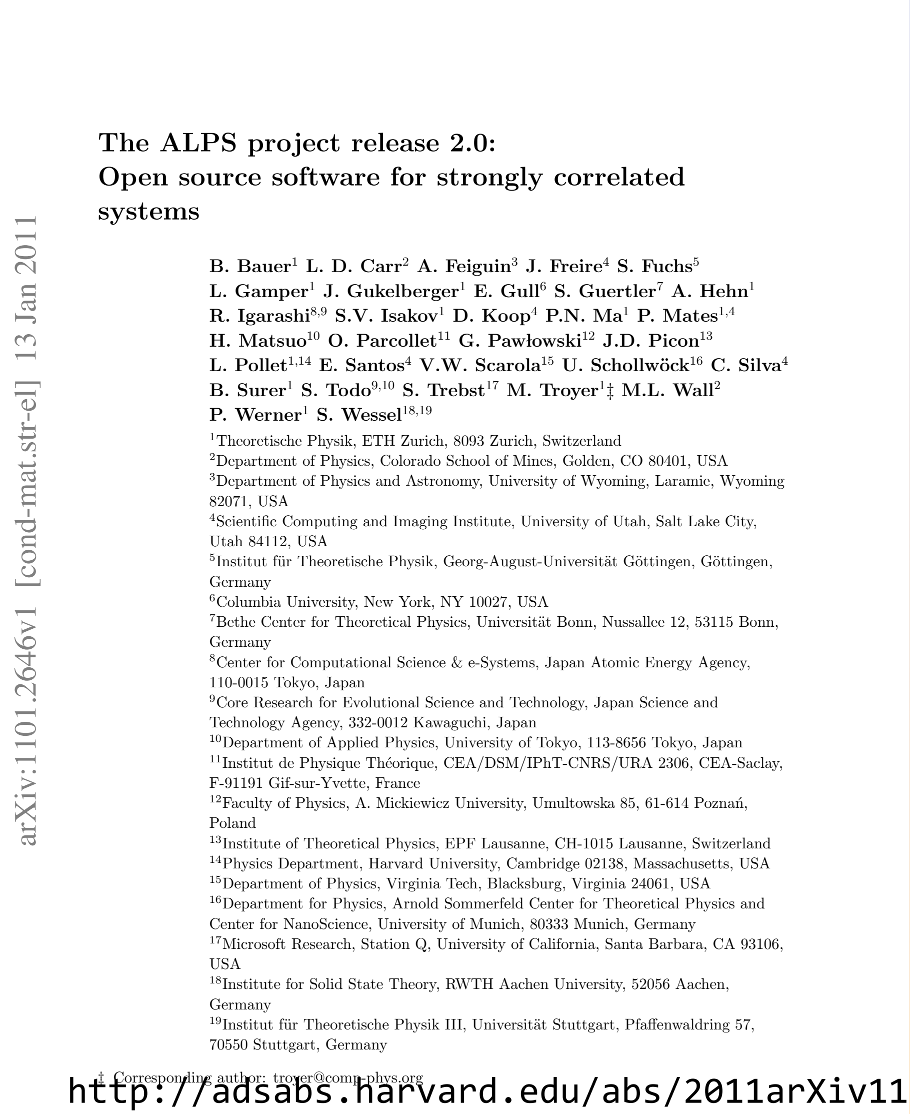


Publication Life Cycle

Our Approach: An Infrastructure to Support Provenance-Rich Papers

- Tools for *authors* to create *workflows* that encode the computational processes, package the results, and link from publications
  - Support different approaches to packaging workflows/data/ environment for publication
- Tools for testers to repeat and validate results
  - How to generate experiments that are most informative given a time/resource limit?
- Interfaces for searching, comparing and analyzing experiments and results
  - Can we discover better approaches to a given problem?
  - Or discover relationships among workflows and the problems?

An *Provenance-Rich* Paper: ALPS2.0



The ALPS project release 2.0:
Open source software for strongly correlated systems

B. Bauer[1] L. D. Carr[2] A. Feiguin[3] J. Freire[4] S. Fuchs[5] L. Gamper[1] J. Gukelberger[1] E. Gull[6] S. Guertler[7] A. Hehn[1] R. Igarashi[8,9] S.V. Isakov[1] D. Koop[4] P.N. Ma[1] P. Mates[1,4] H. Matsuo[10] O. Parcollet[11] G. Pawłowski[12] J.D. Picon[13] L. Pollet[1,14] E. Santos[4] V.W. Scarola[15] U. Schollwöck[16] C. Silva[4] B. Surer[1] S. Todo[9,10] S. Trebst[17] M. Troyer[1]‡ M.L. Wall[2] P. Werner[1] S. Wessel[18,19]

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[4] Scientific Computing and Imaging Institute, University of Utah, Salt Lake City, Utah 84112, USA
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[9] Core Research for Evolutional Science and Technology, Japan Science and Technology Agency, 332-0012 Kawaguchi, Japan
[10] Department of Applied Physics, University of Tokyo, 113-8656 Tokyo, Japan
[11] Institut de Physique Théorique, CEA/DSM/IPhT-CNRS/URA 2306, CEA-Saclay, F-91191 Gif-sur-Yvette, France
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[13] Institute of Theoretical Physics, EPF Lausanne, CH-1015 Lausanne, Switzerland
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[15] Department of Physics, Virginia Tech, Blacksburg, Virginia 24061, USA
[16] Department for Physics, Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, University of Munich, 80333 Munich, Germany
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‡ Corresponding author: troyer@comp-phys.org

http://adsabs.harvard.edu/abs/2011arXiv1101.2646B

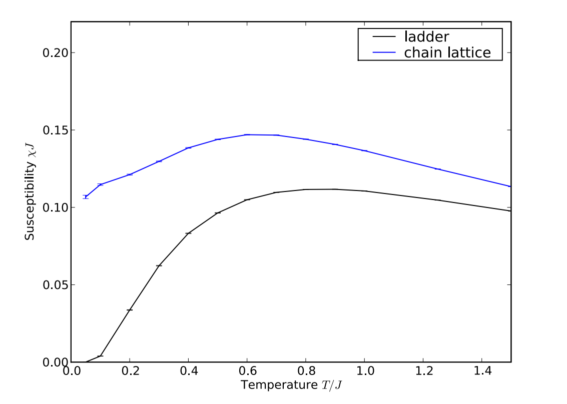
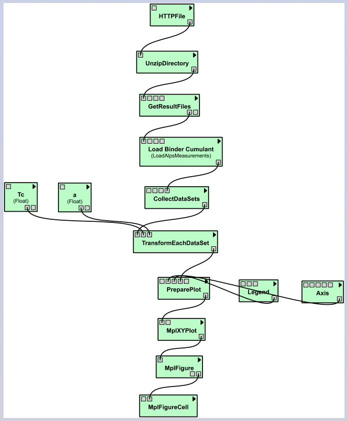
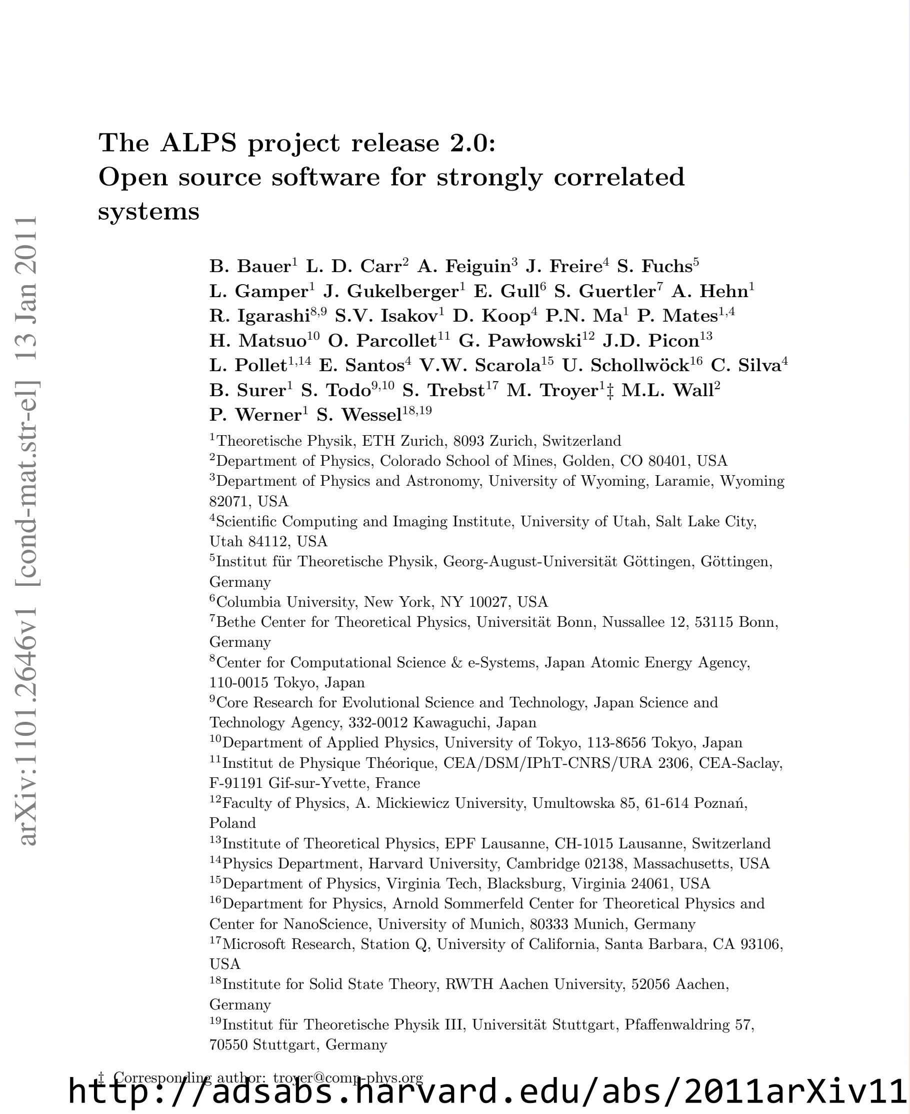


Figure 1. A figure produced by an ALPS VisTrails workflow: the uniform susceptibility of the Heisenberg chain and ladder. Clicking the figure retrieves the workflow used to create it. Opening that workflow on a machine with VisTrails and ALPS installed lets the reader execute the full calculation.



An *Executable* Paper: ALPS2.0



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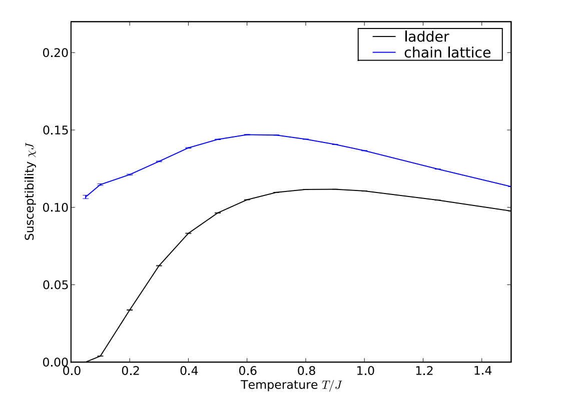

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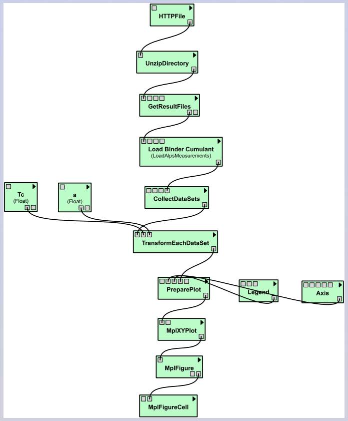


Demo

Editing an executable paper written using LaTeX and VisTrails
http://www.vistrails.org/download/download.php?type=MEDIA&id=executable_paper_latex.mov

Exploring a Web-hosted paper using server-based computation
http://www.vistrails.org/download/download.php?type=MEDIA&id=executable_paper_server.mov

An interactive paper on a Wiki
http://www.vistrails.org/index.php/User:Tohline/CPM/Levels2and3

An Infrastructure to Support Provenance-Rich Papers

- Writing & Development
  - Specifying computations
  - Provenance of data and computations
  - Execution infrastructure
- Review & Validation
  - Local, remote, and mixed execution
  - Interacting, testing and validating computations and their results
- Publishing, Maintenance, & Re-Use
  - Maintenance and longevity
  - Querying and re-using published results.

Writing & Development

An author benefits from working in an environment that simplifies the writing of an executable paper

- Leverage VisTrails' infrastructure

The VisTrails System

- Workflow-based system for data analysis and visualization
- Comprehensive *provenance infrastructure*
- *Transparently* tracks provenance of the discovery process---from data acquisition to visualization
  - The *trail* followed as users generate and test hypotheses
- *Leverage provenance to streamline exploration*
  - Support for reflective reasoning and collaboration
  - Query and mine provenance

•Visualizing environmental simulations (CMOP STC)
•Simulation for solid, fluid and structural mechanics (Galileo Network, UFRJ Brazil)
•Quantum physics simulations (ALPS, ETH Switzerland)
•Climate analysis (CDAT)
•Habitat modeling (USGS)
•Open Wildland Fire Modeling (U. Colorado, NCAR)
•High-energy physics (LEPP, Cornell)
•Cosmology simulations (LANL)

•Study on the use of tms for improving memory (Pyschiatry, U. Utah)
•eBird (Cornell, NSF DataONE)
•Astrophysical Systems (Tohline, LSU)
•NIH NBCR (UCSD)
•Pervasive Technology Labs (Heiland, Indiana University)
•Linköping University (Sweden)
•University of North Carolina, Chapel Hill
•UTEP

Writing & Development

An author benefits from working in an environment that simplifies the writing of an executable paper

- Leverage VisTrails' infrastructure
- Computations specified as workflows
  - Ability to combine tools
  - Support for different levels of granularity can facilitate the understanding of the computations and results
- Provenance of data and computations
  - Parameters, input data, computational environment (OS, library versions, etc)
  - Strong links between data and their provenance [Koop@SSDBM2010]
- Connecting results to their provenance
  - LateX, Word, Powerpoint, HTML, wikis

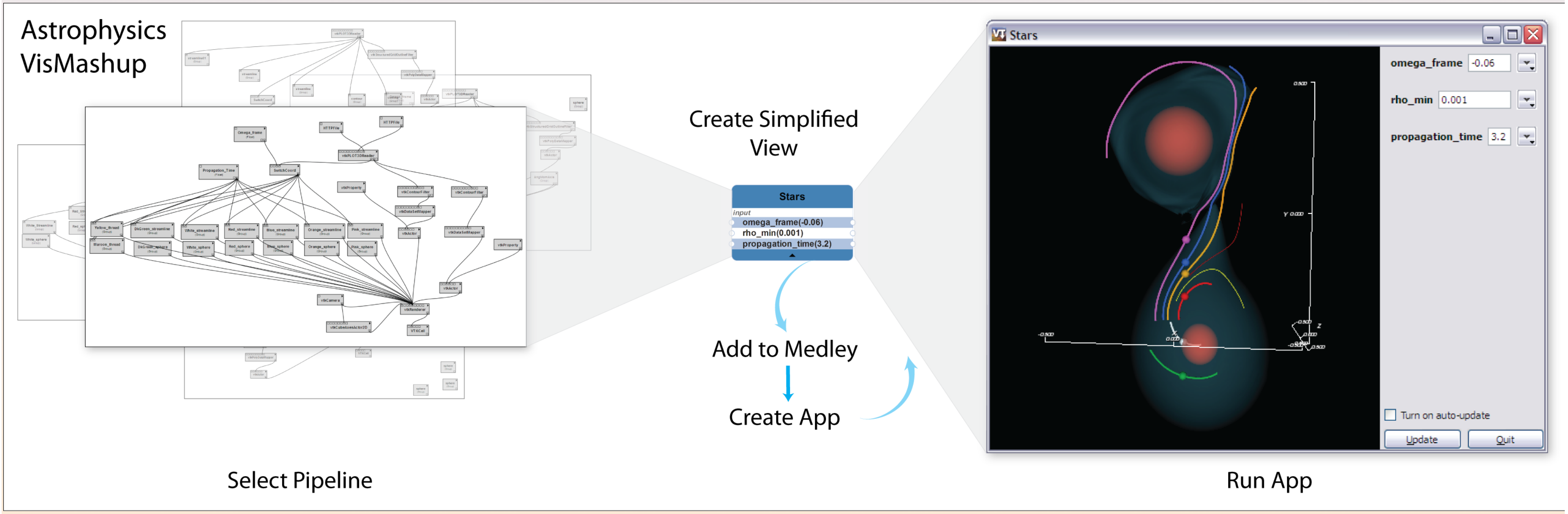
Review & Validation

Improve the quality of reviews: reviewers have the ability to explore and validate conclusions

- Execution environment
  - Software dependencies; proprietary code and data; special hardware
  - Virtual machines, CDEpack
  - Local, remote, and mixed execution
- Testing and validating computations and their results
  - Reproduce
  - Workability: explore parameters and configurations the authors might not have described in the paper
  - Obtain insights
  - Data exploration infrastructure

Publishing, Maintenance, & Re-Use

- Simplify interaction: the VisMashup system [Santos@TVCG2009]



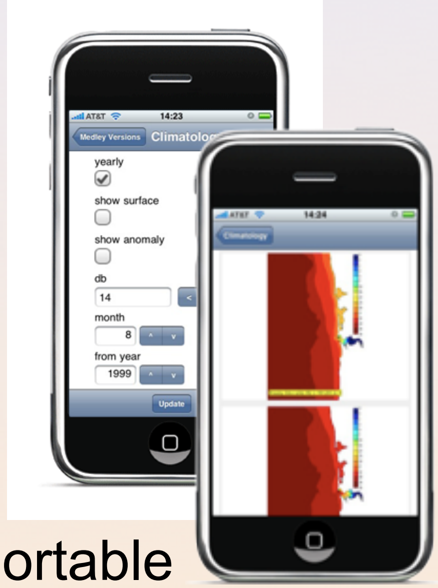
omega_frame(-0.06)
rho_min(0.001)
propagation_time(3.2)

omega_frame -0.06
rho_min 0.001
propagation_time 3.2

Publishing, Maintenance, & Re-Use

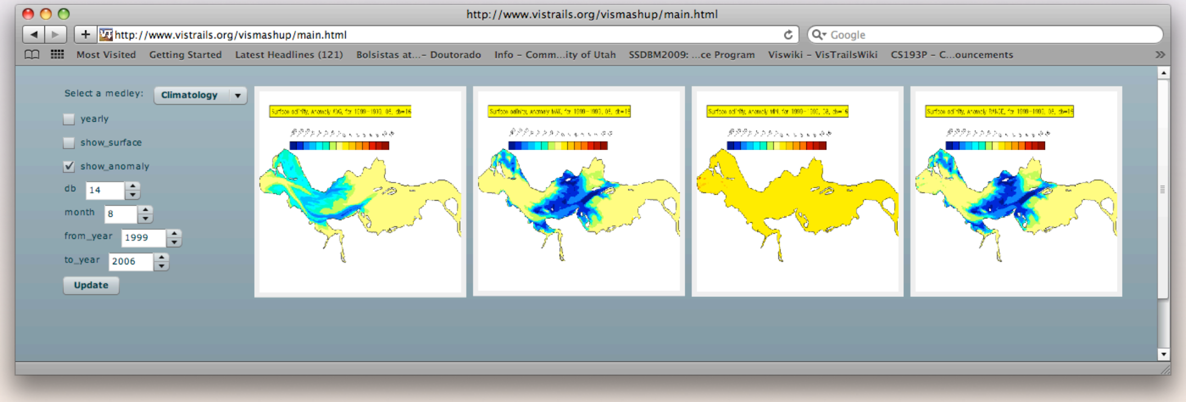
- Simplify interaction: the VisMashup system
- Publish using different media

Web



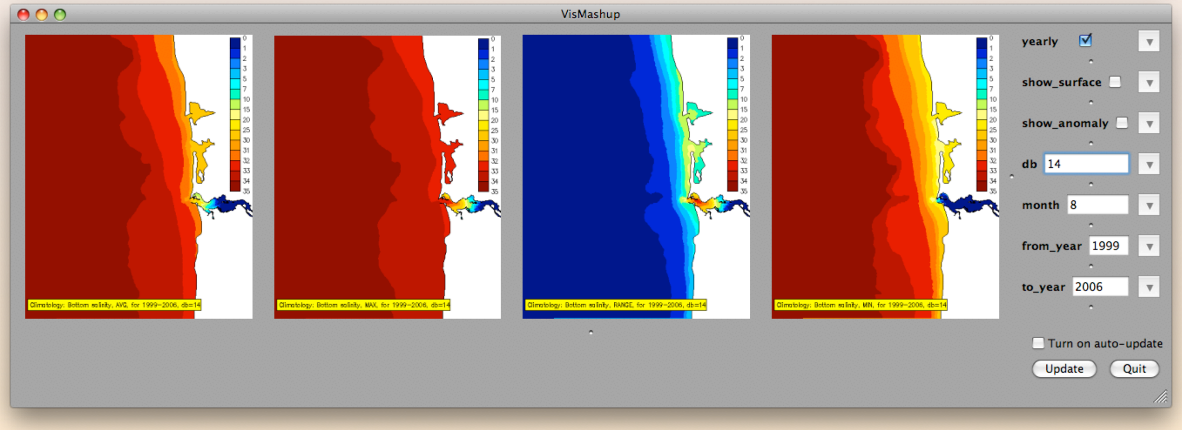
yearly ☑
show surface □
show anomaly □
db 14
month 8
from year 1999
Update

Portable Devices



Select a medley: Climatology

□ yearly
□ show_surface
☑ show_anomaly
db 14
month 8
from_year 1999
to_year 2006
Update


VisMashup
Climatology: Bottom salinity, AVG, for 1999–2006, db=14
Climatology: Bottom salinity, MAX, for 1999–2006, db=14
Climatology: Bottom salinity, RANGE, for 1999–2006, db=14
Climatology: Bottom salinity, MIN, for 1999–2006, db=14
0
1
2
3
5
7
10
15
20
25
30
31
32
33
34
35

yearly ☑
show_surface □
show_anomaly □
db 14
month 8
from_year 1999
to_year 2006
□ Turn on auto-update
Update
Quit

Desktop

Publishing, Maintenance, & Re-Use

- Simplify interaction: the VisMashup system
- Publish using different media
- Maintenance and longevity:
  - Software evolves, try new algorithms: need upgrades [Koop@IPAW2010]
- Querying and re-using published results
  - Opportunities for knowledge discovery and re-use
  - A search/query engine for experiments: text + structure [Scheidegger@TVCG2007]: Can we discover better approaches to a given problem? Or discover relationships among workflows and problems?
  - Combine multiple results through VisMashups

Current Uses

- ALPS community
- Simulations of computational fluid dynamics
- Databases:
  - experiments using distributed database systems, querying Wikipedia
  - http://www.vistrails.org/index.php/RepeatabilityCentral
- ACM SIGMOD repeatability effort
  - Since 2008 verifies the experiments published in accepted papers
  - In 2010, 20% of the papers got the reproducibility stamp!
  - In 2011, use VisTrails and lay out a set of guidelines to simplify and expedite the reviewing process
  - http://www.sigmod2011.org/calls_papers_sigmod_research_repeatability.shtml

Conclusions and Future Work

- Provenance is crucial for science and an enabler for *executable* papers
- Built an end-to-end solution based on VisTrails
  - This is a starting point--many different requirements: need to mix and match different components
  - E.g., it is possible to support for provenance from other tools
- Sharing provenance-rich papers creates new opportunities
  - Expose users to different techniques and tools
  - Users can learn by example; expedite their training; and potentially reduce their time to insight
  - Better science! (remember Tim's Alzheimer's example?)
- Many challenges and several open computer science questions

Acknowledgments

- Thanks to: Philippe Bonnet, Philip Mates, Matthias Troyer, Dennis Shasha, Emanuele Santos, Claudio Silva, Joel Tohline, Huy T. Vo, and the VisTrails team
- This work is partially supported by the National Science Foundation, the Department of Energy, and IBM Faculty Awards.

CMOP
Center for Coastal
Margin Observation
& Prediction

VACET
DOE SciDAC VISUALIZATION AND ANALYTICS
CENTER FOR ENABLING TECHNOLOGIES

THE UNIVERSITY OF UTAH

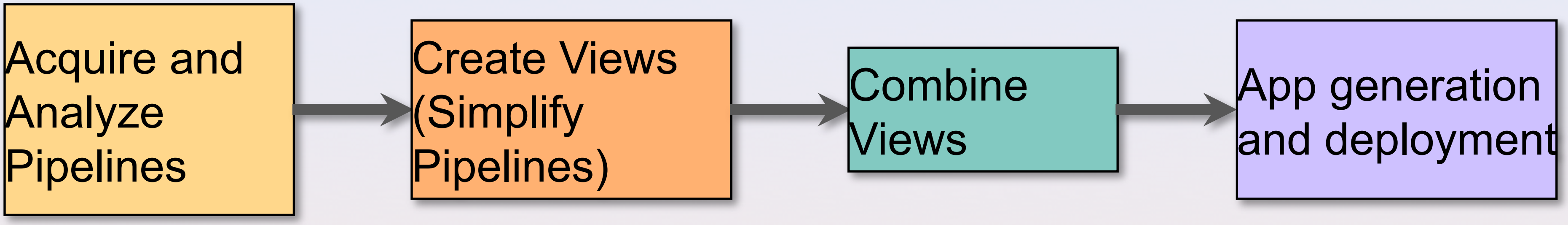
National Science Foundation
WHERE DISCOVERIES BEGIN

SDM CENTER

IBM

Thank you

VisMashup: Creating Mashups from Workflows

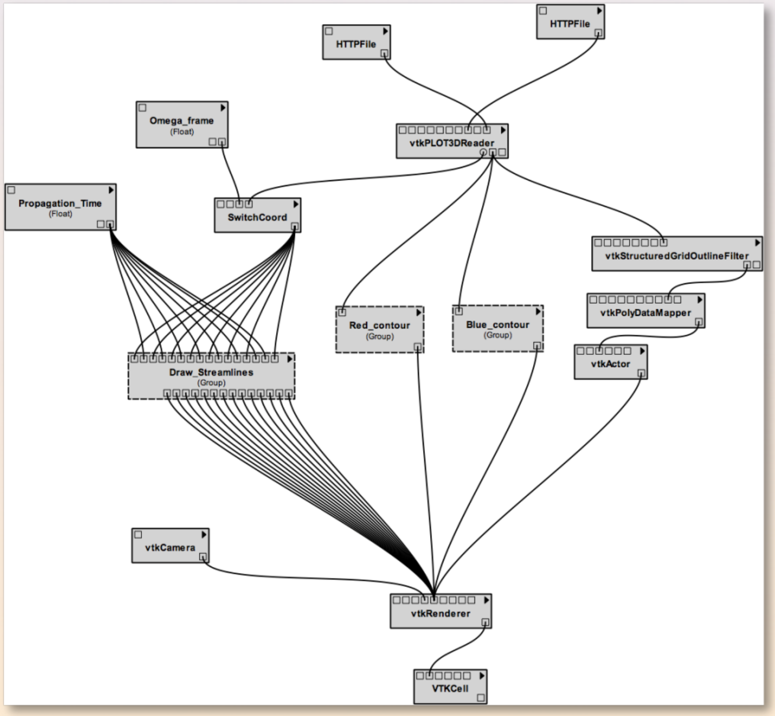


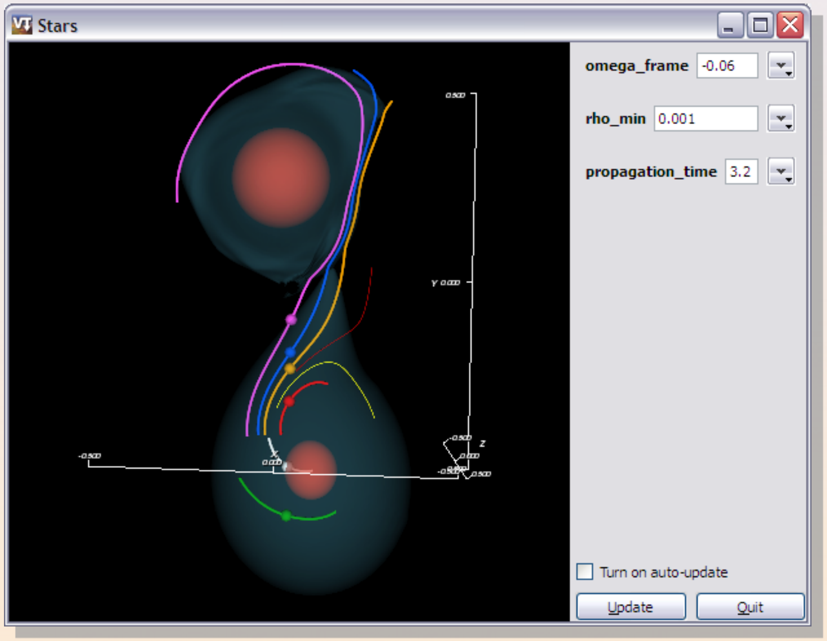
Acquire and Analyze Pipelines

Create Views (Simplify Pipelines)

Combine Views

App generation and deployment





Stars

omega_frame -0.06

rho_min 0.001

propagation_time 3.2

☐ Turn on auto-update

[Santos et al, IEEE TVCG 2008]