UNIVERSITY OF Southampton

Towards a global open scientific notebook infrastructure

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Simon Coles, Colin Bird,
Cerys Willoughby, Cameron Neylon &
Matthew Todd

Science is increasingly interdisciplinary

NATIONAL SCIENCE FOUNDATION
National Science Board
Est. 1950

Digital Research Data Sharing and Management

December 2011

DCC because good research needs good data

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Home > Resources for digital curators > Policy and legal > Overview of funders' data policies

In this section

Briefing Papers

How-to Guides

Overview of funders' data policies

The coverage of funders' publication and data policies

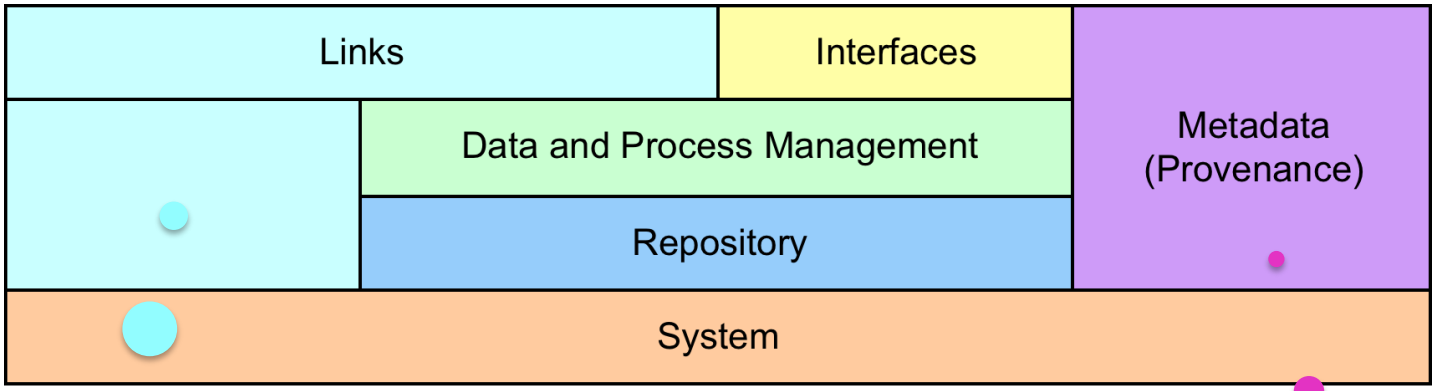
EUROPEAN COMMISSION

PRESS RELEASE

Brussels, 17 July 2012

Scientific data: open access to research results will boost Europe's innovation capacity

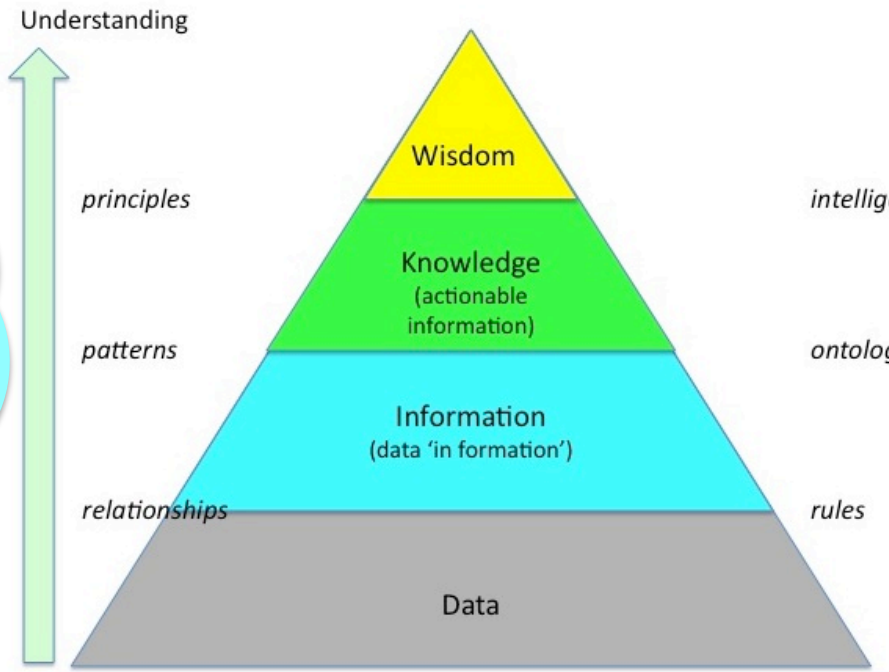
Infrastructures - Architecture



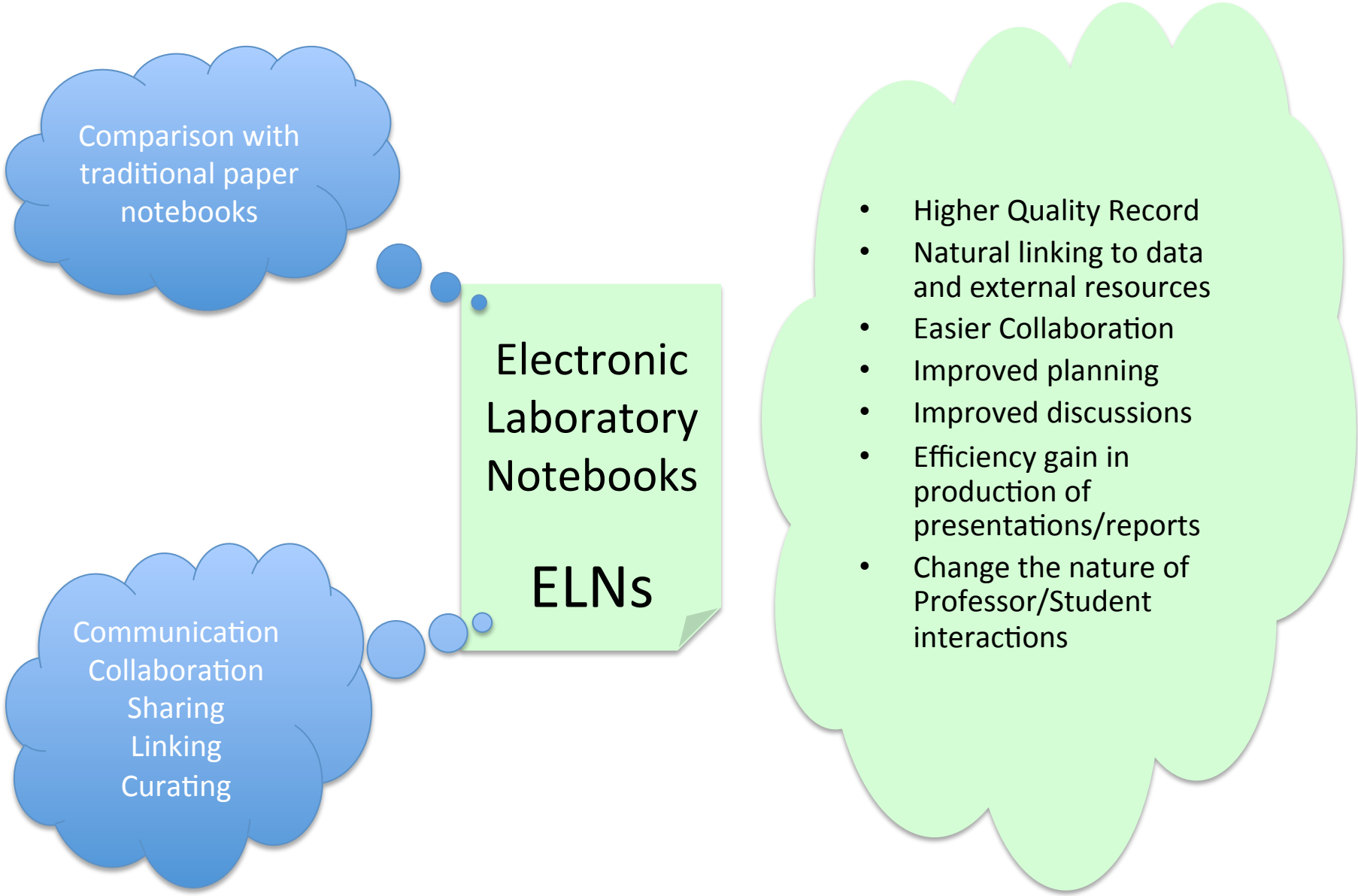
Collaboration

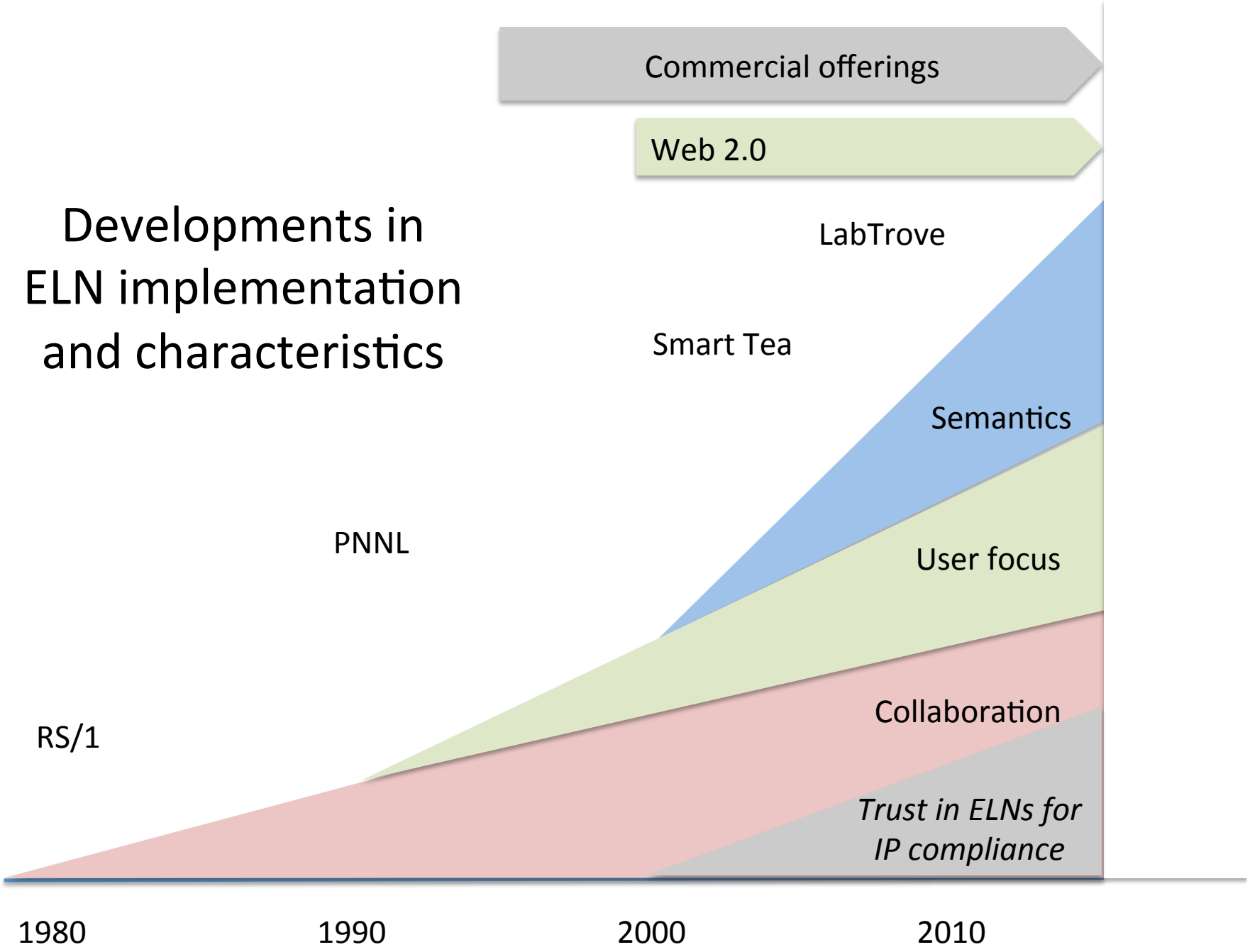
Sharing

Reuse



Curation

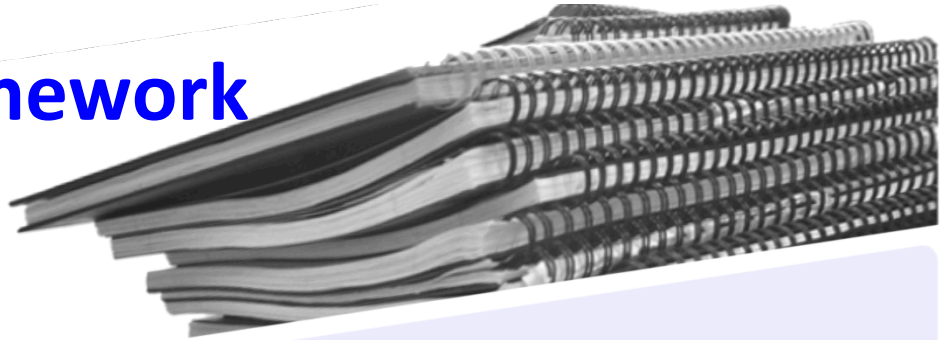

Comparison with traditional paper notebooks
Communication
Collaboration
Sharing
Linking
Curating
Electronic Laboratory Notebooks
ELNs
Higher Quality Record
Natural linking to data and external resources
Easier Collaboration
Improved planning
Improved discussions
Efficiency gain in production of presentations/reports
Change the nature of Professor/Student interactions


Commercial offerings
Web 2.0
Developments in ELN implementation and characteristics
LabTrove
Smart Tea
Semantics
PNNL
User focus
Collaboration
RS/1
Trust in ELNs for IP compliance
1980
1990
2000
2010

The LabTrove story

http://www.labtrove.org

Smart Research Framework



My Lab Notebook

Introduction

- Introduction
- Software Overview
- Partners
- Vision
- SRF Software
  - LabTrove

The SRF project
a shared virtual
management.

Providing tools
to meet the need
responsibility, c
use o
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ental a

SRF

LabTrove

"preserving the record"

flickr.com/julia_manzerova

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ourexperiment

Pictet-Spengler route to Praziquantel

Continuation: Acid-catalyzed Pictet-Spengler reaction with methanesulfonic acid (MW56-9 to MW56-12)

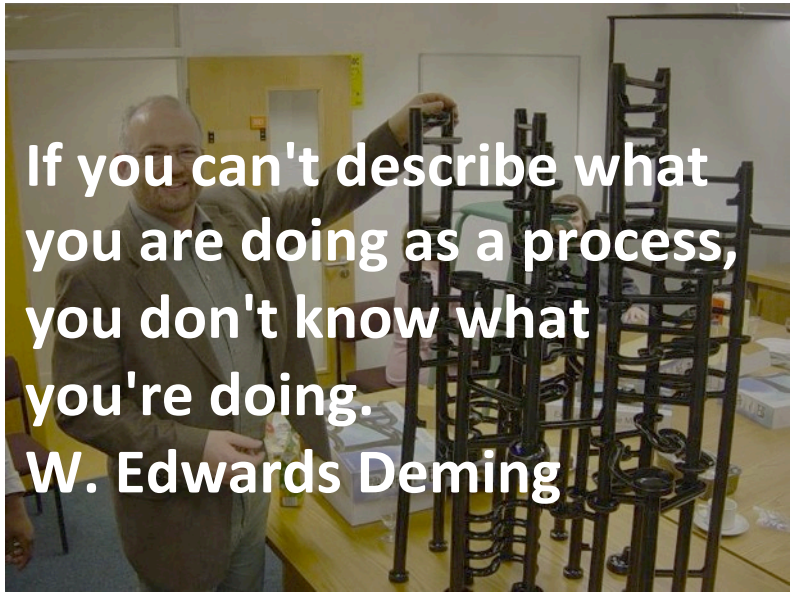
LabTrove
labtrove

labtrove Public Blog Post: Synthesis of amine-linked analogue of TCMDC-123812 via reductive aminatio... http://t.co/Bla5hWbb #malaria #drugdesign
yesterday · reply · retweet · favorite

labtrove Public Blog Post: Synthesis of ether-linked analogue of TCMDC-123812 (PMY 37-1) http://t.co/XhqyRb8i #malaria #drugdesign

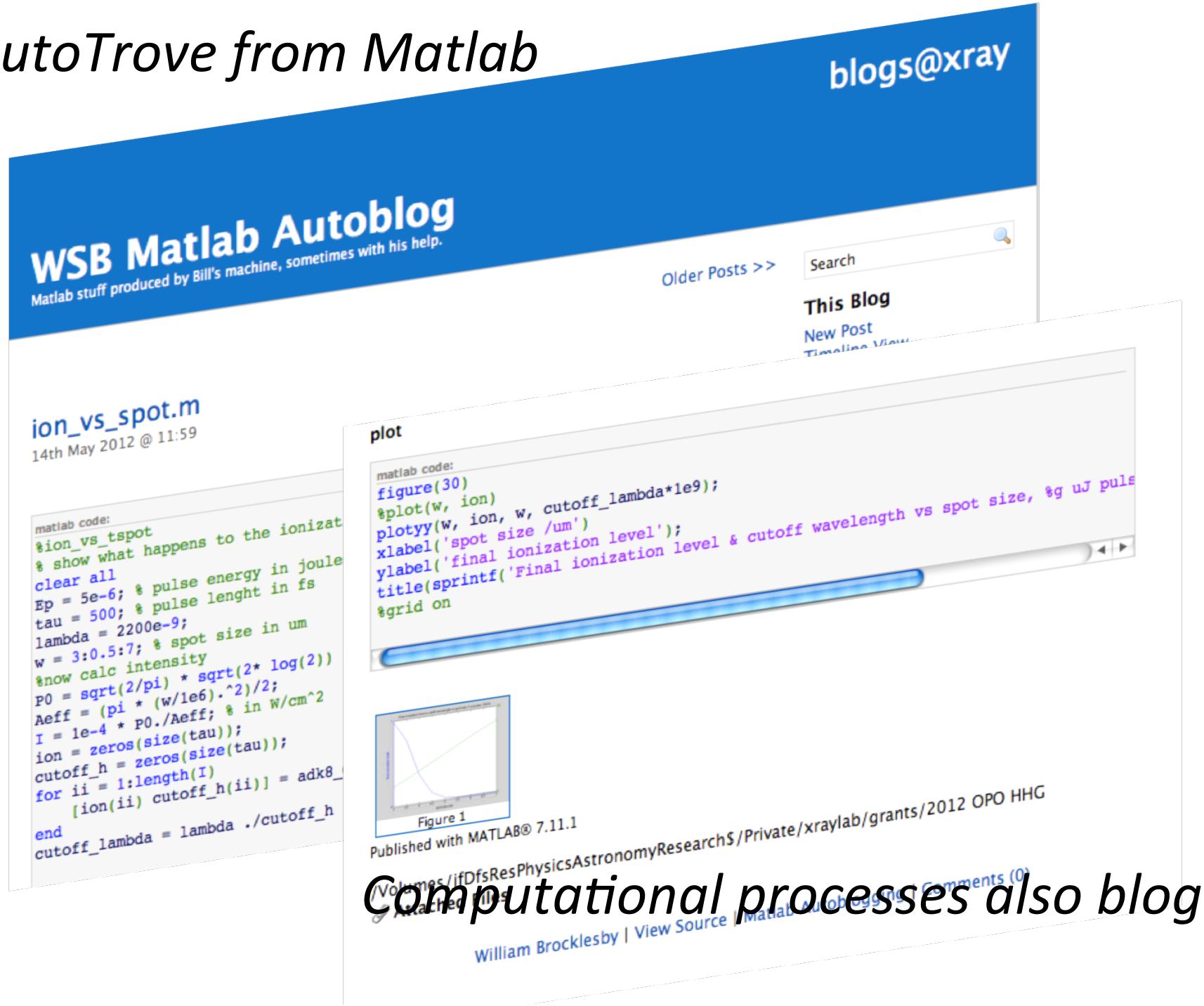
How do we communicate?

- Surprisingly difficult to explain what a process involves
- Much of the detail is assumed to be understood and not explicitly discussed
- This is where the mis-understandings usually arise.



LabTrove: Easy Communication

AutoTrove from Matlab



Computational processes also blog

BlogMyData Project - Godiva

Current user: Andrew Milsted | Log Out

All Blogs | Help

BlogMyData

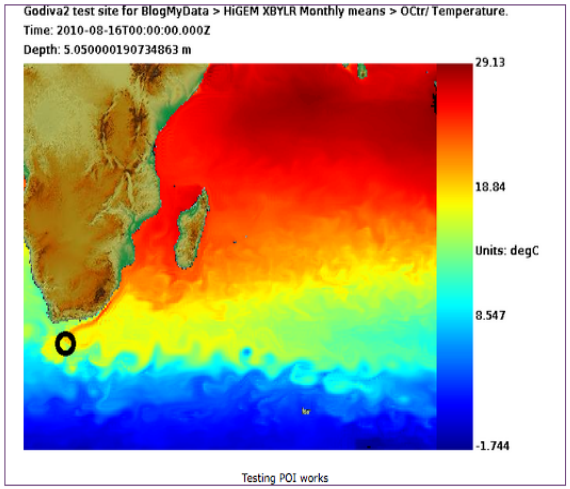
HiGEM Blog

Blog for the HiGEM community

Testing POI works

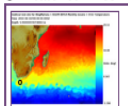
27th August 2010 @ 13:40

Viztype: staticMapWithPoint
Regionofinterest: POINT((21.794815 -38.095867))
Dataset: HIGEM_XBYLR_MONTHLYMEAN
Variableid: temp
Conventions: CF-1.4
Variablestandardname: OCtr/ Temperature.
Variableunits: degC
Bbox: POLYGON((13.359375 -55.689785,95.625 -55.689785,95.625 8.580235,13.359375 8.580235,13.359375 -55.689785))
Crs: EPSG:4326
Time: 2010-08-16T00:00:00.000Z
Calendarsystem: 360_day
Elevation: 5.050000190734863
Elevationunits: m
Elevationpositive: down



ReSC aims to promote e-Science methods in the environmental science community by developing demonstrator projects with collaborators in academia, government agencies (e.g. the Met Office) and industry. These projects will showcase the great potential of e-Science to be a useful method that environmental scientists in many disciplines can use in their everyday research. Tasks that were previously difficult and time-consuming, such as sharing and working with very large data sets, can be made much more efficient.

Attached Files



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HIGEM XBYLR MONTHLYMEAN (13)

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Tools
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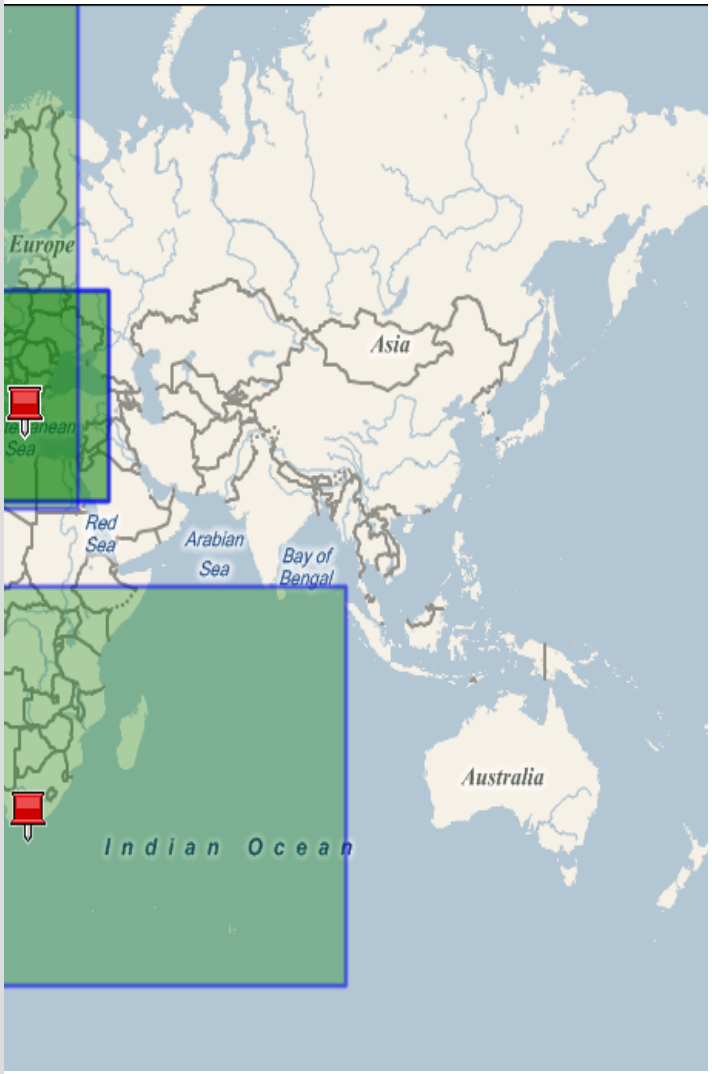
Show/Hide Keys



Light Microscope

UltraFast Xray Group

UNIVERSITY OF Southampton

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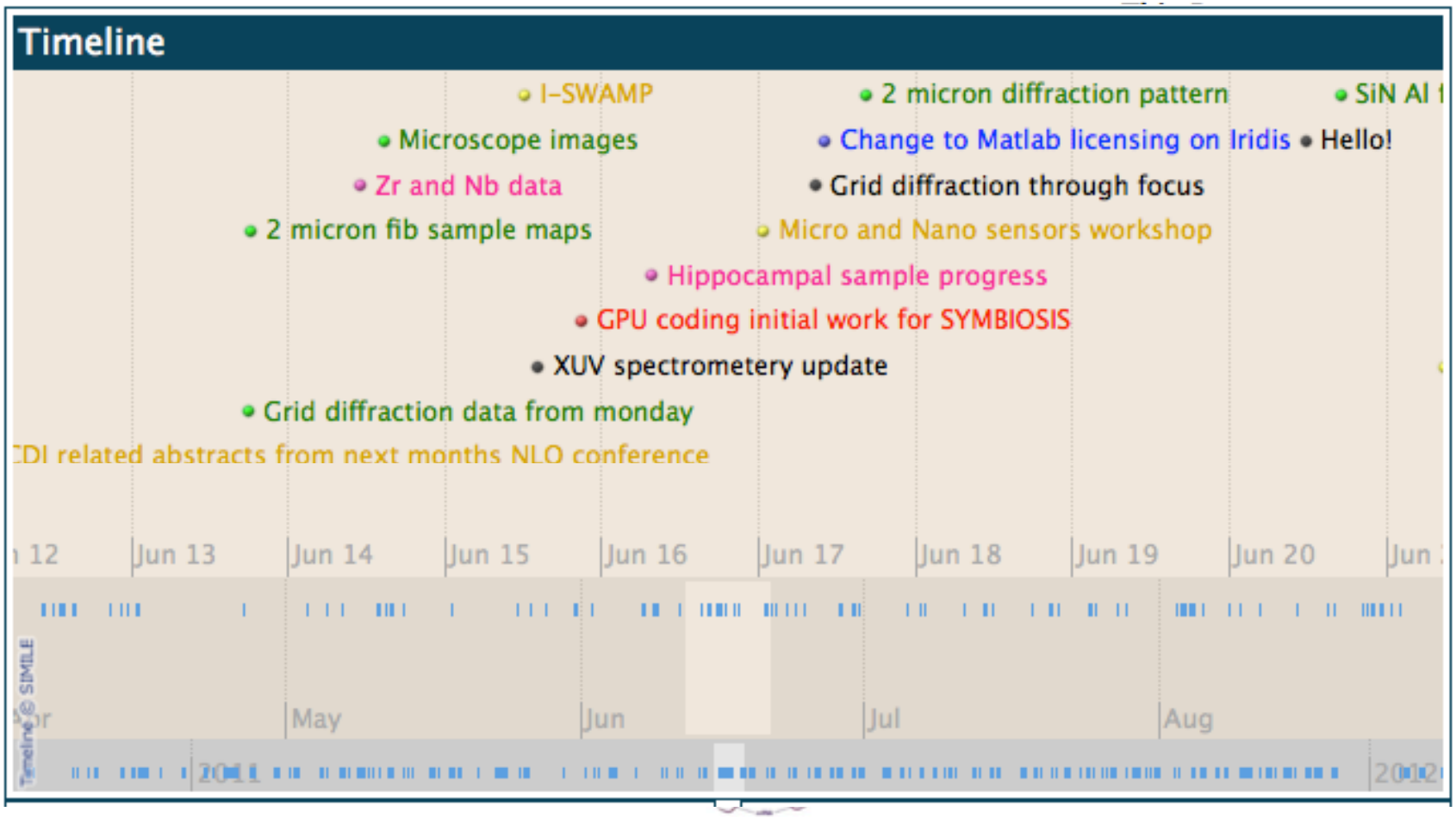
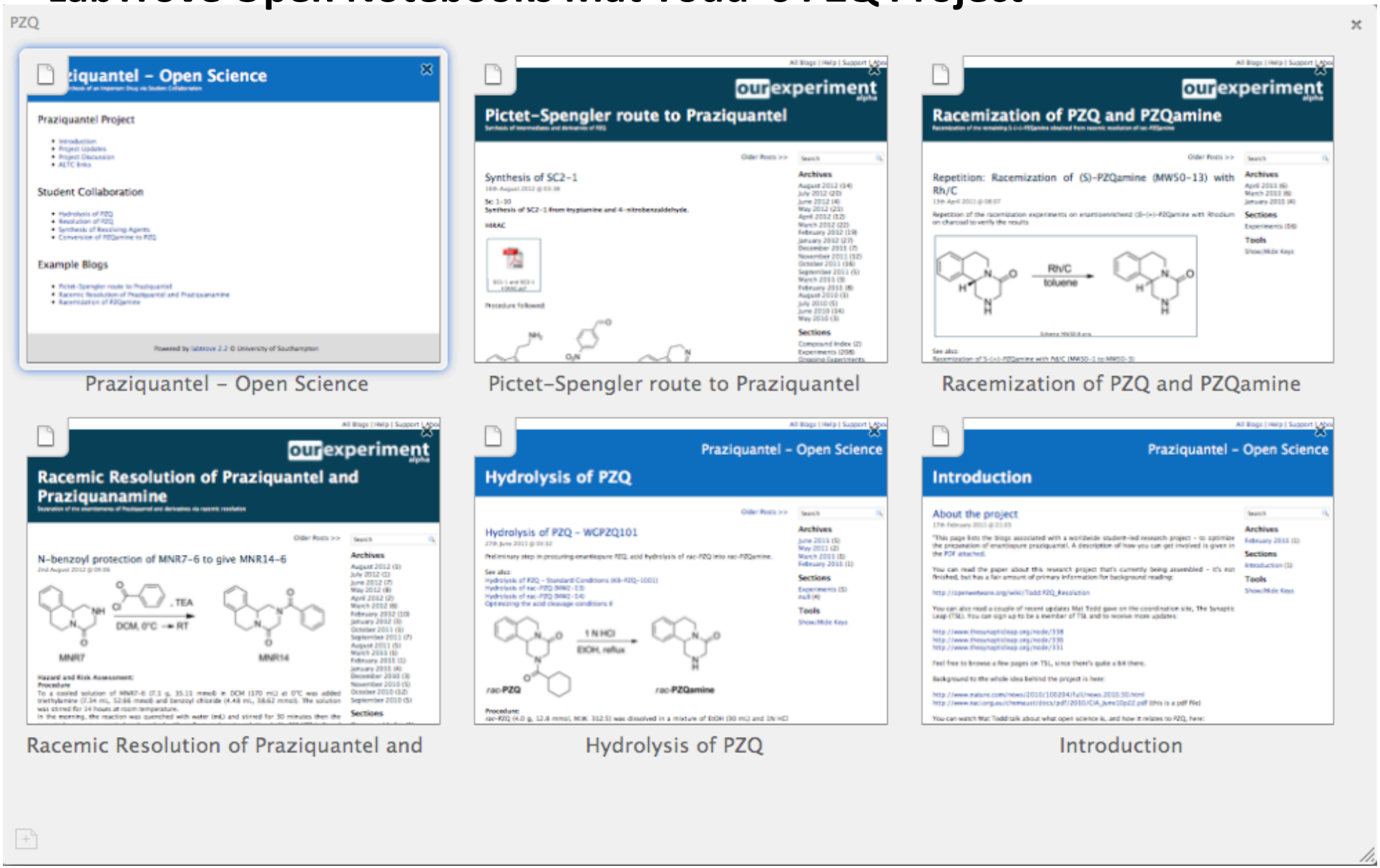


LabTrove Open Notebooks Mat Todd's PZQ Project



Praziquantel – Open Science

Improved Synthesis of an Important Drug via Student Collaboration

Praziquantel Project

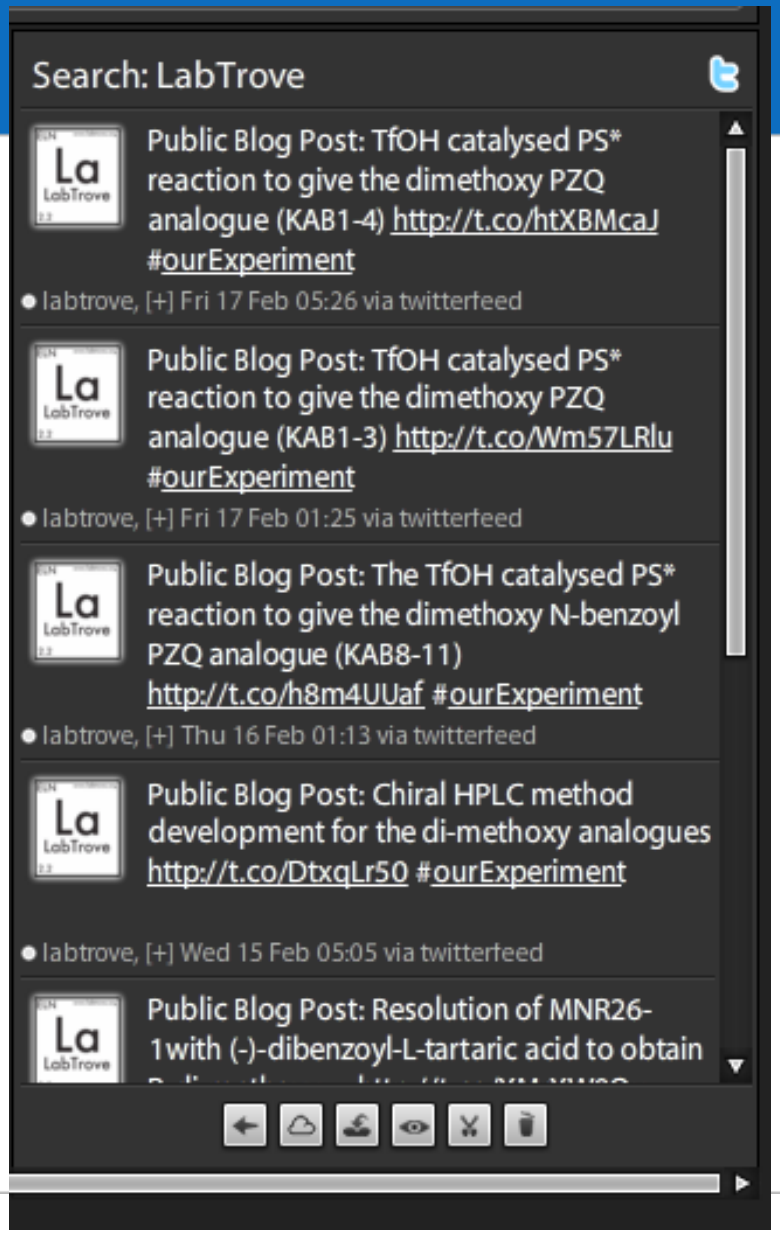
- Introduction
- Project Updates
- Project Discussion
- ALTC links

Student Collaboration

- Hydrolysis of PZQ
- Resolution of PZQ
- Synthesis of Resolving Agents
- Conversion of PZQamine to PZQ

Example Blogs

- Pictet–Spengler route to Praziquantel
- Racemic Resolution of Praziquantel and Praziquanamine
- Racemization of PZQamine

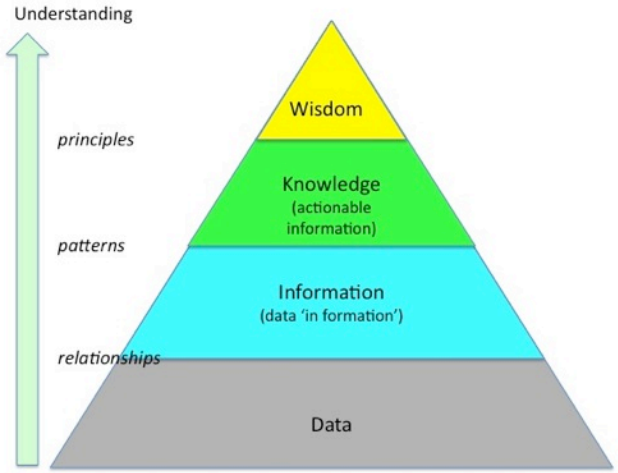


Open Notebooks

- Troves can be open Read/Comment/Write
  - Can control this access so it is your choice
- All contributions attributable (login needed)
  - Anonymous contributions not usually enabled
- Open contribution does worry the IT services
  - Provides potential pathway for abuse of systems
  - Not just our systems

Global open scientific notebook infrastructure

- Global collaboration:
  - International
  - Interdisciplinary
- Open science



- To ascend the *knowledge pyramid*, we need open collaboration and sharing of results

We must speed up the knowledge discovery process

All I am saying is that now is the time to develop the technology to deflect an asteroid