A Universal Identifier for Computational Results

AAAS 2011

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March 4, 2011
Credibility Crisis in Scientific Communication

Jon Claerbout, 1990 (paraphrase Donoho and Buckheit, 1995)

An article about computational science in a scientific publication is not the scholarship itself, it is merely advertising of the scholarship. The actual scholarship is the complete software development environment and the complete set of instructions which generated the figures.

• “Most published scientific research is false”. (John Ioannidis, with apologies)
• “Most published scientific research is not reproducible”. (John Ioannidis et al., Keith Baggerly et al.)
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Stages of Reproducibility

- Write scientific paper [1660?]
- Publish a pidgin algorithm and describe simulation datasets [1950?]
- Sell magtape of code and data [1970?]
- Place idiosyncratic software at website.
  - Place idiosyncratic dataset at Website [1991?]
- Write R Package, of software, place at CRAN.
  - Publish datasets and scripts at Website [2000?]
- Use Sweave to integrate code and data [??]
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Encouraging signs –

- *Biostatistics* has a reproducibility editor (*Roger Peng*), standard process for certification (using R)
- Growing literature on reproducibility (Special issues, workshops like this one, …)

The truth is –

- Very few researchers follow even minimal reproducibility standards.
- No-one expects or requires reproducibility [Even my own students!]
- No uniform standards of reproducibility, so no established user base.
Reflections 1...

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Psychological Obstacles to Reproducibility

- Publication is the real goal
- Publication is *informal* description of work we do in *private*
- We use files and personal coding idioms *no-one else will ever see*
- Reproducibility involves cleaning up post-facto. It’s a *pretentious waste of time*.

Working reproducibility requires a discipline

- *The endgame*. Release of code and results to the internet.
- Commit to the endgame *before you start your project*
- Work consistently to a discipline *shaped by the endgame*
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Claerbout’s motto, again

An article about computational science in a scientific publication is not the scholarship itself, it is merely advertising of the scholarship. The actual scholarship is the complete software development environment and the complete set of instructions which generated the figures.
Operational meaning of the motto

We describe an approach, implemented in software, which makes the following a reality:

- Running a computational experiment necessarily ends in publication of the computational process and its results in a public repository.
- Writing explanations related to computational results (e.g., a scientific article advertising it) is done afterwards, or not at all.
- Figures in article are renderings of the already published computational results.
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Claerbout’s motto - Operational meaning

An article about computational science is not the scholarship itself, it is advertisement captions written around renderings of previously published Verifiable Computational Results (VCRs). The actual scholarship is the complete VCR record on a public repository, containing a complete account of the computational process which generated the figures.
Publication and Computation are one and the same

- Every computation for a scientific project, at instant of creation, is *publicly registered* (+timestamped, documented) at *external server*.
- URI generated by registration makes result *eternally* and *universally* accessible *.
- Scientific Publication is post-facto creation of humanly-readable hypertext document explaining *pre-existing, already ‘public’ results*.
- No computational result is citable *unless at instant of its creation it was appropriately registered*.
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Problem we’ve encountered

1. How exactly did I create this nice figure two years ago?

My own paper
Problem we’ve encountered

2. My student Bob graduated. My new student Alice can't reproduce his thesis results.

Bob’s thesis
3. I don’t believe the figure in this published paper.
Problem we’ve encountered

4. I don’t believe the figure in your lecture slide.
Problem we’ve encountered

5. I cannot honestly referee this paper without the computation details.

A Submitted paper

Red: original, Blue: recovered from M=200 samples.
Red: original. Blue: recovered from M=200 samples.

URI: vcr.stanford.edu/fmmfda-6ec4-5664-8290-b40cf3ae0d16
(Try clicking on the figure...)
vcr.stanford.edu/fffffffda-6ec4-5664-8290-b40cf3ae0d16
is a URI: Universal Result Identifier

URI is a universal and permanent connection to a computational result (and its generating environment)
vcr.stanford.edu/ffffffffda-6ec4-5664-8290-b40cf3ae0d16 is a URI: Universal Result Identifier

URI is a *universal* and *permanent* connection to a computational result (and its generating environment)
The computational science workflow

Program Code

```python
x = read_data('C:/result_of_previous_computation.txt')
figure1 = plot(x)
save(figure1,'figure1.eps')
```

Document processor

```
\includegraphics{C:/figure1}
```

Publication: Paper or slides
The computational science workflow

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Document processor

```latex
\includegraphics{C:/figure1}
```

Publication: Paper or slides

![Graph showing post-origign: Blue recovered from 600 samples](C:/figure1)
How computational science used to work

Program Code

```matlab
function experiment

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> experiment
> "C:/figure1.eps saved"
How computational science used to work

Document processor

...Our results are summarized in Figure 1.
\includegraphics{C:/figure1}
How computational science used to work

Publication: Paper or slides

...Our results are summarized in Figure 1.
How computational science *should* work

**Program Code**

```plaintext
function experiment

    repository('vcr.science.com')
    x = read_data('vcr.science.com/cd6e83d7-3929')
    verifiable figure1 = plot(x)
```
How computational science should work

Program Code

function experiment

    repository('vcr.science.com')
    x = read_data('vcr.science.com/cd6e83d7-3929')
    verifiable figure1 = plot(x)

> experiment
How computational science *should* work

**Program Code**

```python
function experiment

    repository('vcr.science.com')
    x = read_data('vcr.science.com/cd6e83d7-3929')
    verifiable figure1 = plot(x)

> experiment
> "vcr.science.com replied:"
> "URI of figure1 is ffaaffb1-48d7"
> "Receipt sent to gavish@stanford.edu"
```
How computational science should work

...Our results are summarized in Figure 1.
\include_result{vcr.science.com/ffaaffb1-48d7}
How computational science *should* work

Publication: Paper or slides

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(Try clicking on the figure...)

URL: vcr.stanford.edu/ffm3a-6ec4-5564-8290-b40cf3ae6d16
Eventual system components
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The bottom line

Using our system requires -
- Publishers to make subtle changes in article appearance
- Authors to make simple changes in a few lines of programs and word processors

Using our system allows/implies -
- Universal, permanent and secure identifier for each citable computational result
- A single, citable copy of each published result
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- Immediate publication * of result upon issuance of URI
- VCR server protocol serves up not only result, but various views and metadata about result
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  Dataset values, summaries
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New Psychology (encore)

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({{gavish,donoho}@stanford.edu}) Universal Result Identifiers March 4, 2011 28 / 31
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Web Services Standards

- URI – Universal Resource Identifier
- RESTful web service (e.g., Amazon S3)

Implications

- Instead of files, objects in the cloud.
- Server responds to object/method pairs
- URI: http://www.stanford.edu/ gavish/vcr/371aae2f-0d1f-405b-f1dd-7d4446363324
- URI+method: http://www.stanford.edu/ gavish/vcr/371aae2f-0d1f-405b-f1dd-7d4446363324(row=3,col=21)
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- URI: http://www.stanford.edu/gavish/vcr/371aee2f-0d1f-405b-f1dd-7d4446363324
- URI+method:
  http://www.stanford.edu/gavish/vcr/371aee2f-0d1f-405b-f1dd-7d4446363324/row=3/col=21
 Larger Picture – Computational Results are Web Services

Web Services Standards

- URI – Universal Resource Identifier
- RESTful web service (eg Amazon S3)

Implications

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Existing implementation

Beta version in use in the Stanford Statistics Department.
http://vcr.stanford.edu
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