Introduction to Reproducible Research

Quantitative Fisheries Center, Michigan State University

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Reproducible Research

- Philosophical
  - reproducibility is one of core principles of the scientific method
  - some consider reproducible research to be the gold standard in scienetific credibility as all of the data, analsyses and reports are encaspulated in a single entity
  - some journals are moving towards reproducibility standards (e.g. see: http://biostatistics.oxfordjournals.org/content/10/3/405.full)

Reproducible Research

An article about computational science in a scientific publication is not the scholarship itself, it is merely advertising of the scholarship.

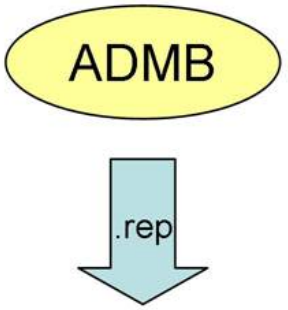
The actual scholarship is the complete software development environment and the complete set of instructions which generated the figures

- Professor Jon Claerbout
  Stanford University
  - source:http://www.rrplanet.com/reproducible-research/reproducible-research.shtml

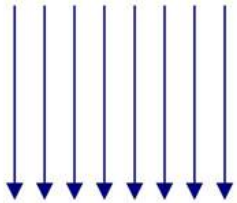
Reproducible Research

- From a more practical perspective:
  - reproducible research means being able automatically recreate your reports when data is changed or updated
  - or recreating your exact working directory to a state that generated a specific report, presentation or result

Typical Work Flow



- separate files for each stage of process:
  - data cleaning and preparation
  - model fitting and analysis
  - summarization and reporting
- lots of clicking and copy-paste
- often uses proprietary binary file format (.ppt, .doc, .xls) that is difficult to 'version'
- tedious, error prone, difficult or impossible to replicate exactly



But what if . . .

- I make a small change to data?
- I have multiple reports?
- I want to implement complicated model improvements that might break everything?
- I need to find data and exact model or source code that created a specific report
- I need to work collaborative with an other analyst?
  - How do I know **exactly** what's changed?
  - How do I integrate their changes with my changes?

Reproducible Research

- provides an alternative method of work that avoids many of these problems
- Literate Programing
- Donald Knuth
- more recently...

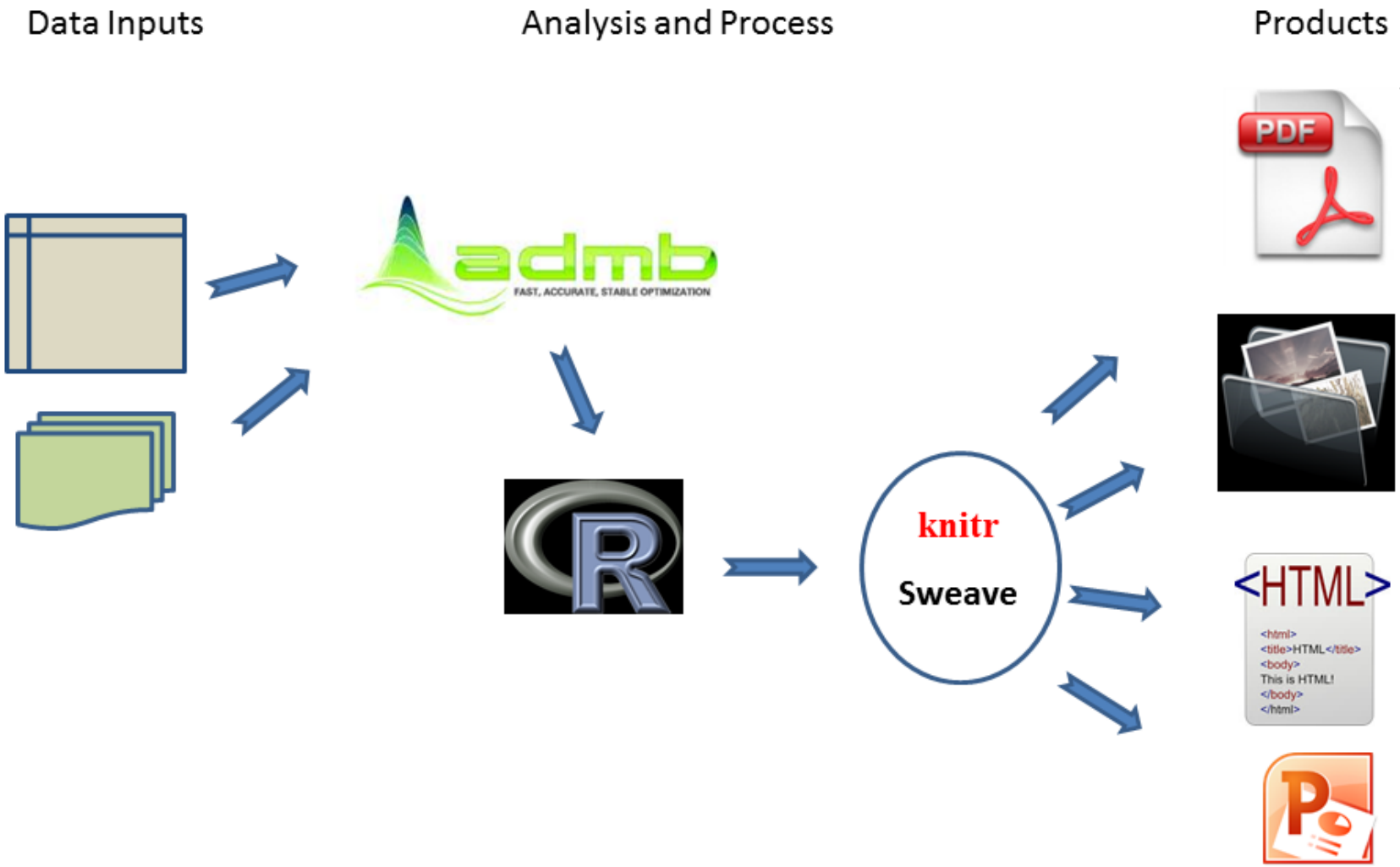
An Alternative Work-flow

- all preparation, analysis, reporting done in simple text files
- results from analysis integrated directly into source code for reporting products - reports, presentations, html documents
- reports automatically regenerated when data changes
- no undocumented figures, tables or results

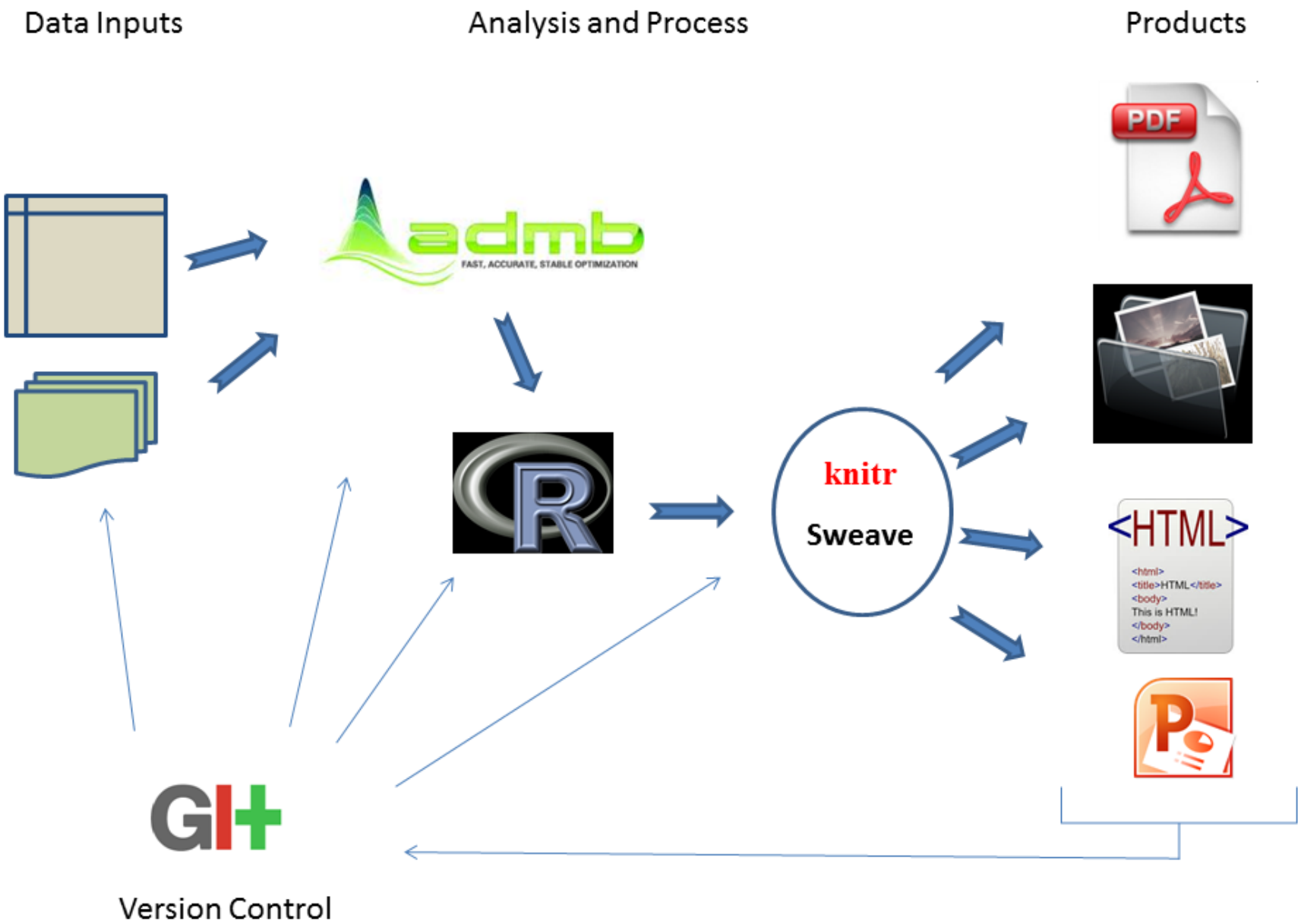
An Alternative Work-flow (cont'd)

- no undocumented clicking or cutting and pasting
- version control software keeps track of changes
  - reset directory to past states
  - compare changes from one state to another
  - branching and merging allow 'safe' development

An Alternative Work-flow (cont'd)



An Alternative Work-flow (cont'd)



10 Simple Rules

From (Sandve et al. 2013): [1]

- For Every Result, Keep Track of How It Was Produced
- Avoid Manual Data Manipulation Steps
- Archive the Exact Versions of All External Programs Used
- Version Control All Custom Scripts
- Record All Intermediate Results, When Possible in Standardized Formats

[1] Sandve GK, Nekrutenko A, Taylor J, Hovig E (2013) Ten Simple Rules for Reproducible Computational Research. PLoS Comput Biol 9(10): e1003285. doi:10.1371/journal.pcbi.1003285

10 Simple Rules (cont'd):

From (Sandve et al. 2013): [2]

- For Analyses That Include Randomness, Note Underlying Random Seeds
- Always Store Raw Data behind Plots
- Generate Hierarchical Analysis Output, Allowing Layers of Increasing Detail to Be Inspected
- Connect Textual Statements to Underlying Results
- Provide Public Access to Scripts, Runs, and Results

[2] Sandve GK, Nekrutenko A, Taylor J, Hovig E (2013) Ten Simple Rules for Reproducible Computational Research. PLoS Comput Biol 9(10): e1003285. doi:10.1371/journal.pcbi.1003285

Further Reading and Resources

- Oxford Scientific Journals:

http://biostatistics.oxfordjournals.org/content/10/3/405.full

- R's Reproducible Research Task page:

http://cran.r-project.org/web/views/ReproducibleResearch.html