ACCELERATING SYNTHESIS SCIENCE THROUGH REPRODUCIBLE SCIENCE PRACTICES

Matthew B. Jones

National Center for Ecological Analysis and Synthesis University of California Santa Barbara



@metamattj
jones@nceas.ucsb.edu
https://orcid.org/0000-0003-0077-4738





Ecological Synthesis



Marine Systems



Threats and Population Declines



Understanding Ocean Health



Climate and Ecosystems











Reproducible Science



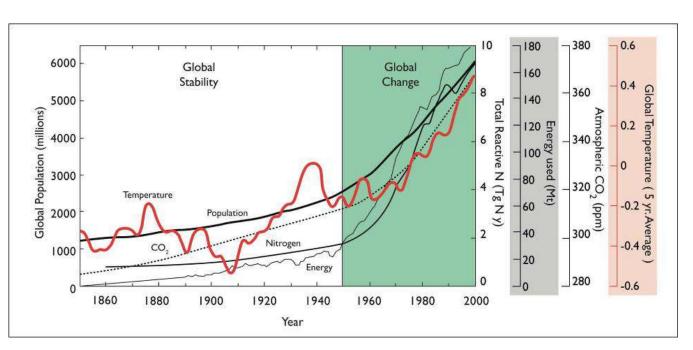
Climate Change Fisheries Sustainabiity Subsistence

Science Governance Regulation Policy





Trust in Science



What data? What methods? What parameter settings?

Can we **trust** these data and methods?

Smith et al. (2009) Ecology doi:10.1890/08-1815.1

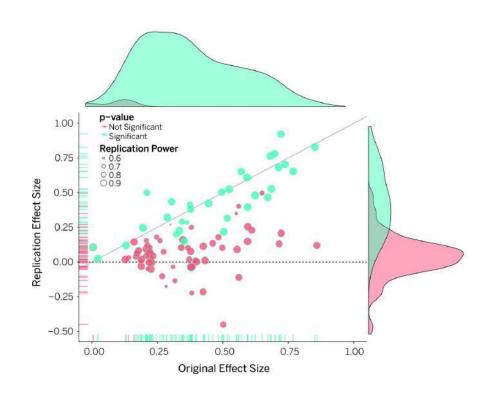
Reproducibility Crisis

"Most research findings are false for most research designs and for most fields"

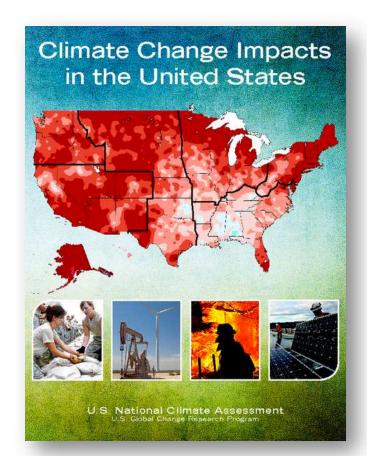
Ioannidis, 2005

"Most replication effects were smaller than original results"

Open Science Collaboration, 2015



National Climate Assessment



"This report is the result of a three-year analytical effort by a team of over 300 experts, overseen by a broadly constituted Federal Advisory Committee of 60 members. It was developed from information and analyses gathered in over 70 workshops and listening sessions held across the country."

Computational Reproducibility

Facilitate transparency by capturing and communicating scientific workflows

Stand on the shoulders of giants (build on work that came before)

Increase trust in science



Give credit for that **secondary** usage enabling **easy attribution**

Practical Reproducibility



Preserve the software workflow

Document what you did

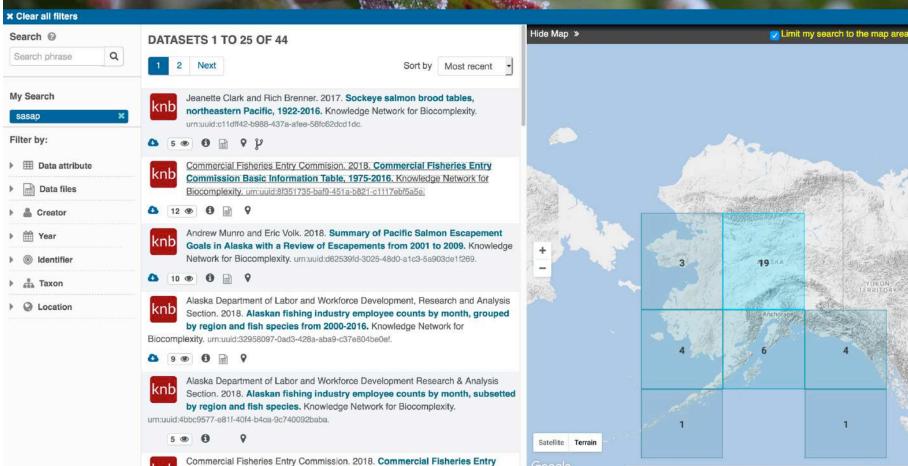
Describe how to interpret it all







KND ABOUT DATA SHARE TOOLS Jump to: DOI or ID Go SIGN IN



Map data @2018 Google, INEGI, SK telecom, ZENRIN 500 km L....

■ Terms of Use

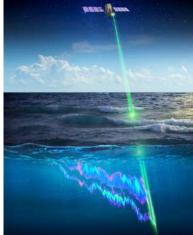


https://search.dataone.org



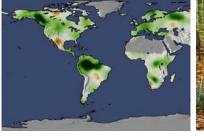


800KData Packages













40Repositories



143KContributors





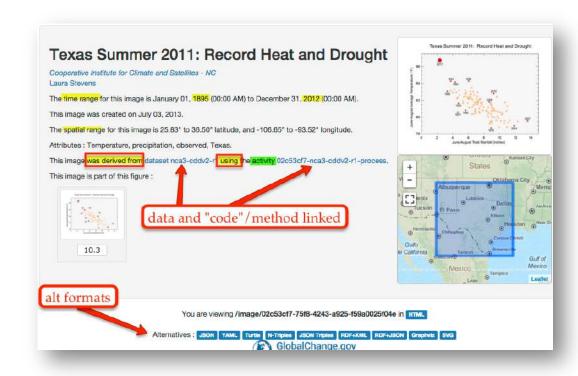




Computational Provenance

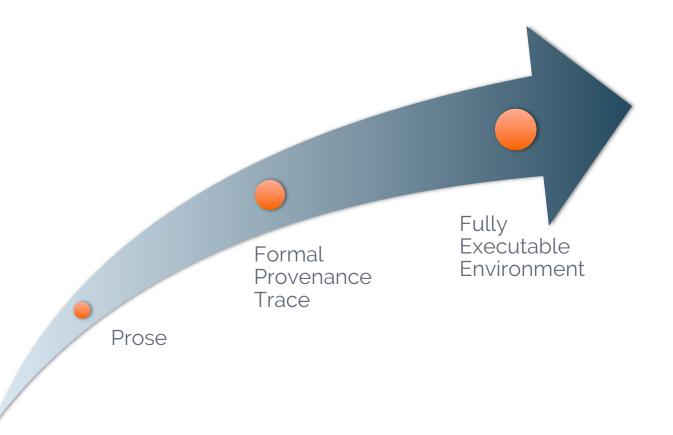
Origin, processing history of data

- Input data
- Workflow/scripts
- Output data
- Figures
- Understand methods, dataflow, and dependencies



Provenance

Origin and processing history of artifacts



Provenance in DataONE

Phase II Goal: Facilitate reproducible science

- Track data derivation history
- Track data inputs and outputs of analyses
- Track analysis and model executions
- Preserve and document software workflows
- Link all of these to publications

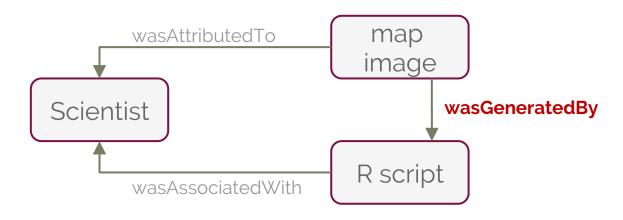
Provenance for Science Workflows

ProvSNE

ProvONE – an extension of W3C PROV

See purl.dataone.org/provone-v1-dev





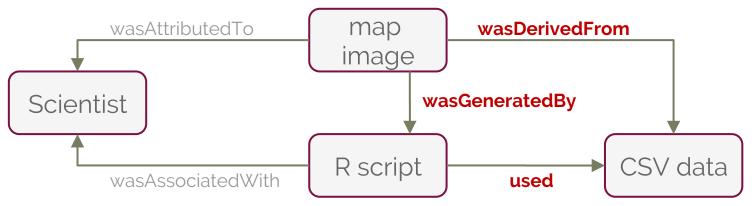
Provenance for Science Workflows

ProvSNE

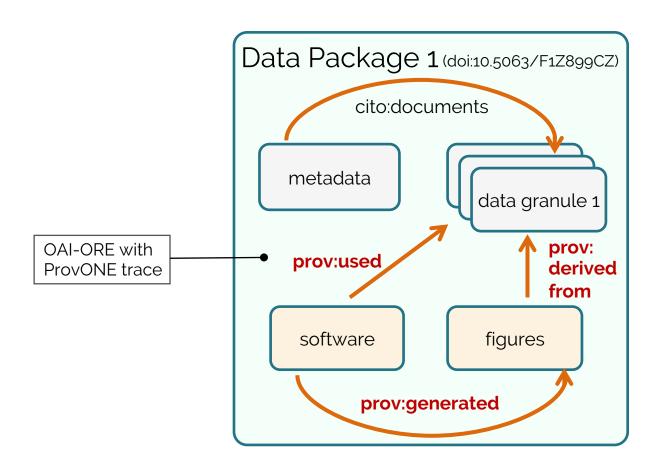
ProvONE – an extension of W3C PROV

See purl.dataone.org/provone-v1-dev



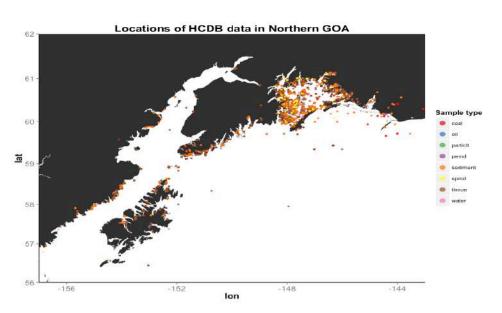


Data Package with Provenance

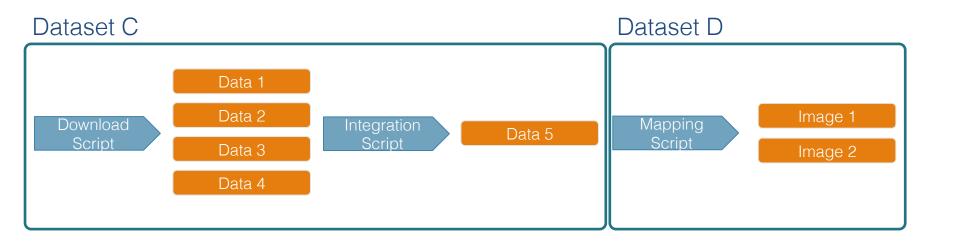


Hydrocarbon Data Example

Mark Carls. 2017. Analysis of hydrocarbons following the Exxon Valdez oil spill, Gulf of Alaska, 1989 - 2014. Arctic Data Center.



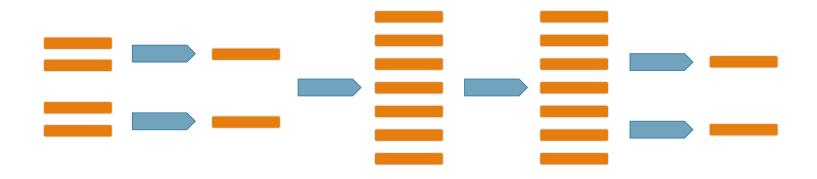
Publishing Data Workflows



Hydrocarbon Data Example

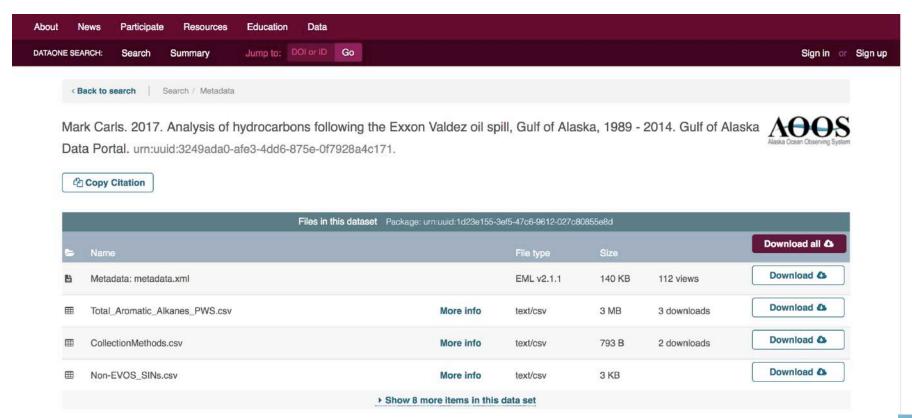
Complex Workflows

Simplified view of complex workflows

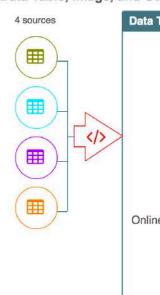


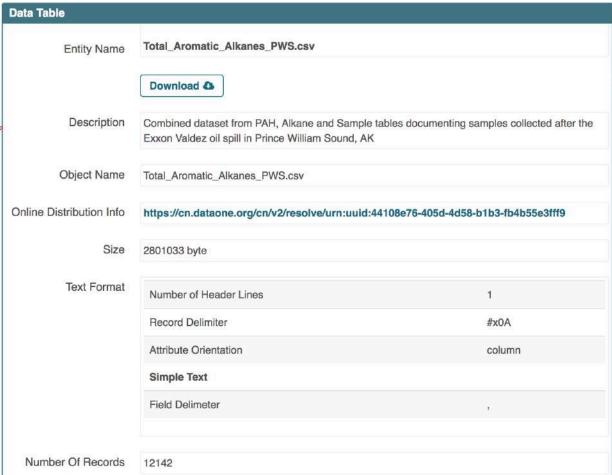
Provenance Display

DataONE Search

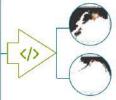


Data Table, Image, and Other Data Details

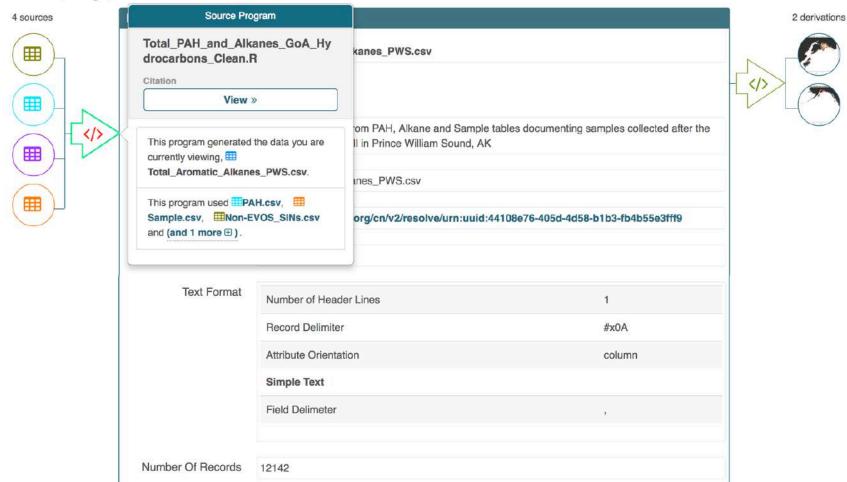




2 derivations

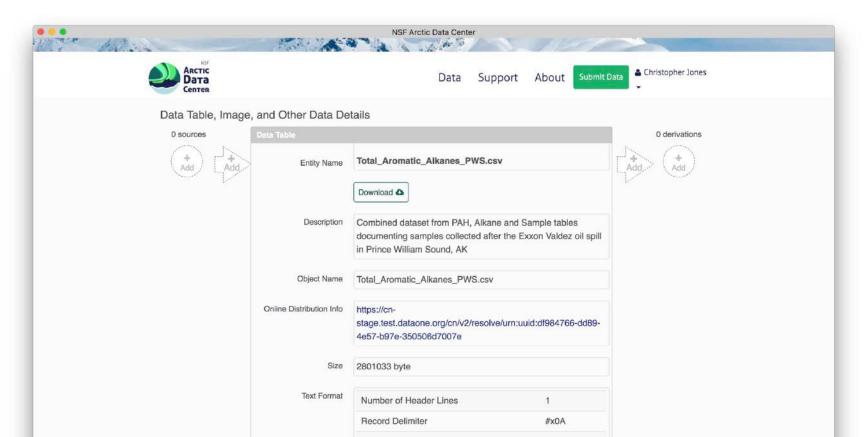


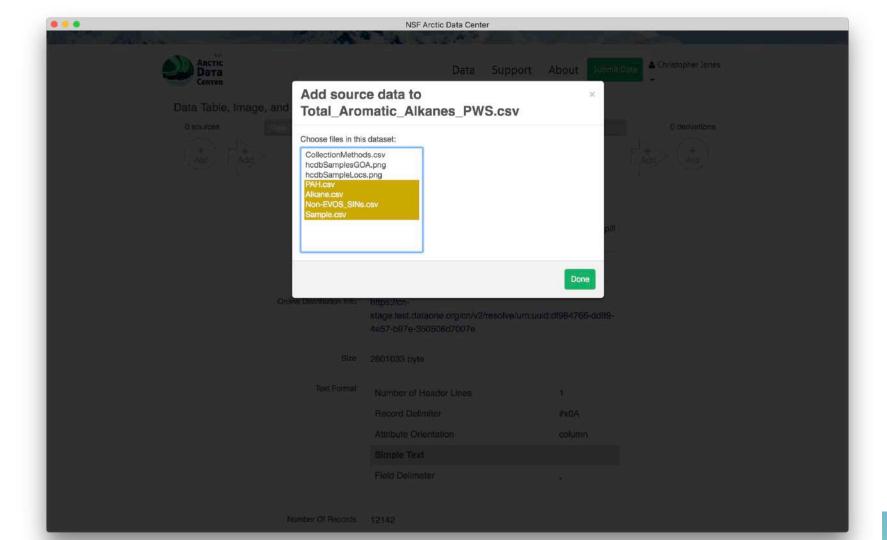
Data Table, Image, and Other Data Details

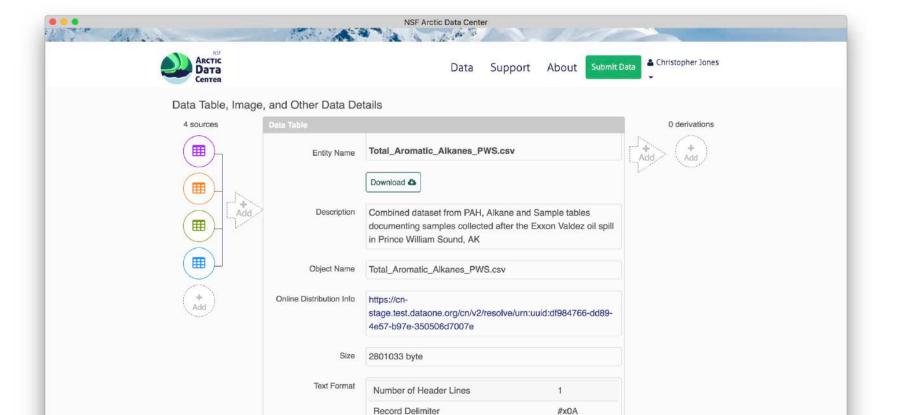


Web Provenance Editor

Deployed by Arctic Data Center







Attribute Orientation

Simple Text Field Delimeter column

Provenance Editing



Matlab DataONE Toolbox



Recordr R Library



YesWorkflow Tool

MetacatUI Web Provenance Editor











Credit where credit is due

Indexing and exposing data citations in international data repository networks











Force11 Data Citation Principles

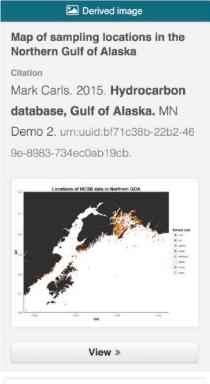
- 1. Importance of data citation
- 2. Credit and Attribution
- 3. Evidence
- 4. Unique Identification
- 5. Access
- 6. Persistence
- 7. **Specificity** and Verifiability
- 8. Interoperability and Flexibility

Transitive Credit

When a user cites a pub, we know:

- Which data produced it
- What software produced it
- What was derived from it
- Who to credit down the attribution stack

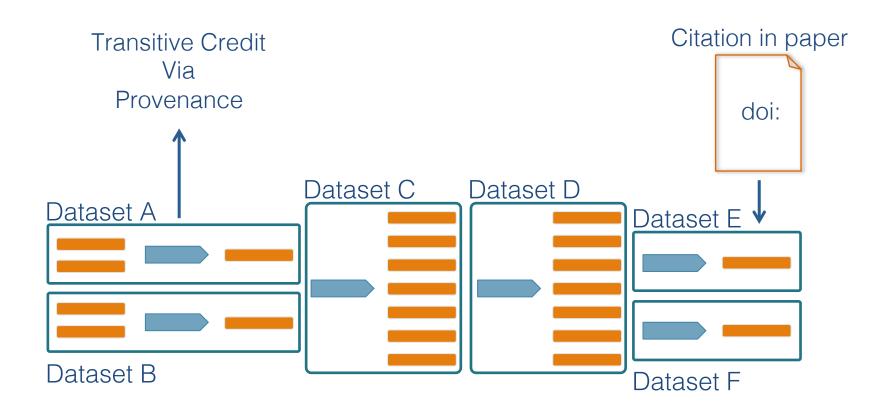
See: Katz & Smith. 2014. Implementing
Transitive Credit with JSON-LD. arXiv:1407.51



This image was generated by the program you are currently viewing, Locations map R script .

This image was derived from
Total_Aromatic_Alkanes_PWS.csv .

Citing multi-generational workflows



Evolution of the Living Paper



Scholarly Publications

1 st Gen	Prose		
2 nd Gen	Prose	+ Data	
3 rd Gen	Prose	+ Data	+ Code



Prose + Data + Code + Provenance



Prose + Data + Code + **Provenance + Execution Environment**





Theoretical and Applied Climatology

November 2016, Volume 126, <u>Issue 3-4</u>, pp 699–703 | <u>Cite as</u>

Learning from mistakes in climate research

Authors and affiliations Authors

Rasmus E. Benestad , Dana Nuccitelli, Stephan Lewandowsky, Katharine Hayhoe, Hans Olav Hygen, Rob van Dorland, John Cook

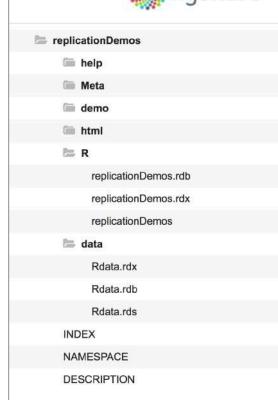
Open Access Original Paper

First Online: 20 August 2015



Downloads Citations





Ships with an R package





Edzer Pebesma

@edzerpebesma



Replying to @jhollist @metamattj

It is on CRAN, but in Archived; I could install it after installing a bunch of other Archived packages from source, and could run a number of examples. Another number depended on web resources no longer available.

5:04 AM - 14 Jul 2019



Parsing Reproducibility

- Empirical Reproducibility:
 - traditional empirical experiments, e.g. at the bench/lab
- Statistical Reproducibility:
 - statistical methodology used permits generalizability of data inferences
- Computational Reproducibility:
 - transparency of computational steps that produce scientific findings

Simplifying Computational Reproducibility in Whole Tale



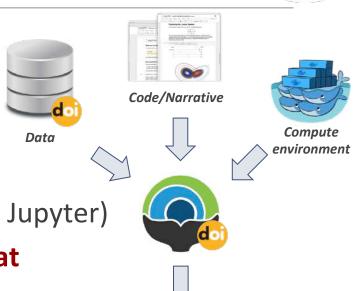
- Researchers can easily package and share tales:
 - O Data, Code, and Compute Environment
 - to re-create the computational results from a scientific study
 - achieving computational reproducibility
 - thus "setting the default to reproducible."
- Also empowers users to verify and extend results with different data, methods, and environments.

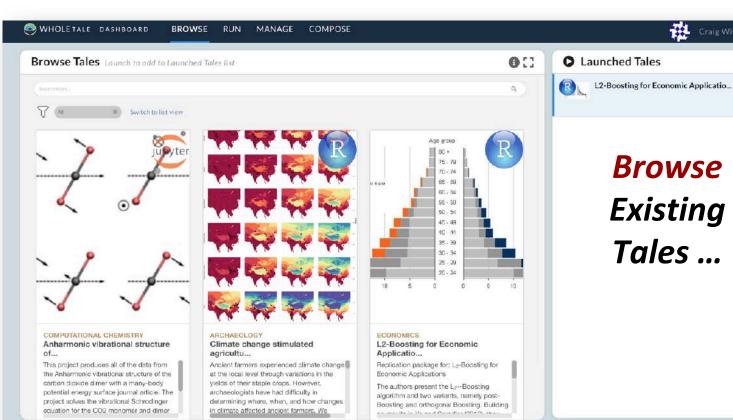
V. Stodden, D. H. Bailey, J. Borwein, R. J. LeVeque, W. Rider, and W. Stein. (2013). Setting the Default to Reproducible: Reproducibility in Computational and Experimental Mathematics, ICERM workshop (2013)



What exactly is (in) a Tale?

- Tale = executable research object, i.e.
 - data (references)
 - + code (computational methods)
 - + narrative (traditional science story)
 - + compute environment (e.g. RStudio, Jupyter)
- Captured in a standards-based tale format complete with metadata





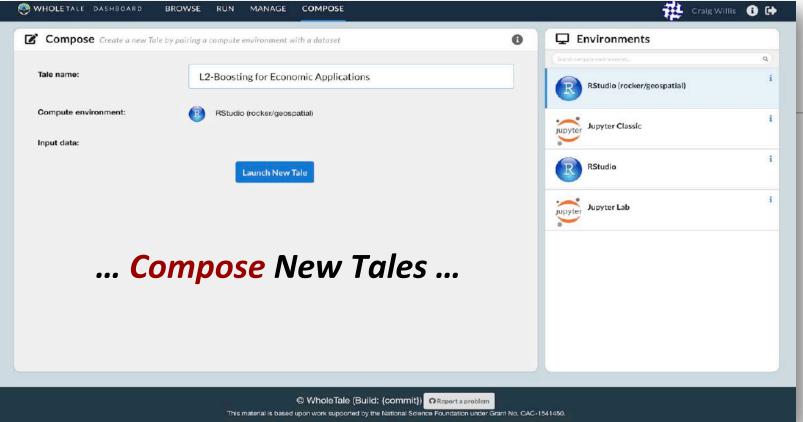


Existing Tales ...

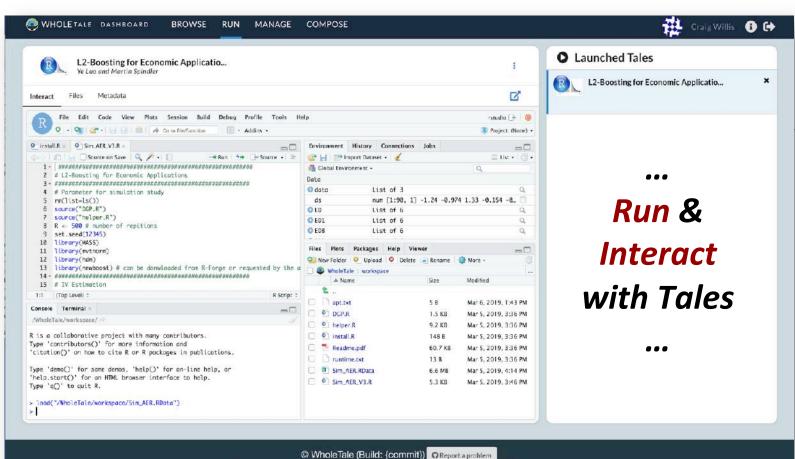
Craig Willis 🕕 😝

×

This material is based upon work supported by the National Science Foundation under Grant No. OAC-1541450.

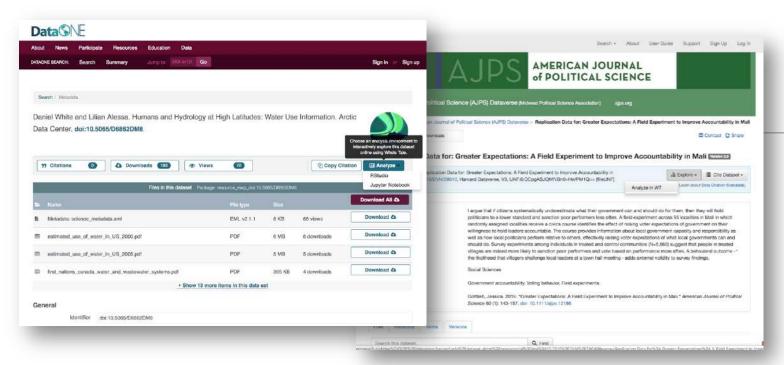






This material is based upon work supported by the National Science Foundation under Grant No. OAC-1541450.







... Integrate Data Repos with Whole Tale!

- Enables turnkey exploratory data analysis on existing published datasets
- DataONE and Dataverse networks cover > 90 major research repositories!





Publish Tale Publishing will create an immutable copy of your Tale with a DOI. This process will allow another user to easily rerun your published analysis using the WholeTale platform. Please choose a target repository: * DataONE-The Knowledge Network for Biocomplexity More Details * Your published Tale will include everything that has been uploaded to its associated workspace. The following required files will be generated and published along with the Tale itself: Quantifying FAIR: metadata improvement and guidance in the DataONE repository network manifest.json 0 environment.json (1) LICENSE (1) README.md (1) metadata.xml 0 This process will allow another user to easily rerun your published analysis using the WholeTale platform. For more information about publishing, please consult the Publishing Guide. Cancel **Publish**

... Publish Data, Code, and Environment

 Enables full circle reproducibility to
 DataONE repositories that accept API deposits

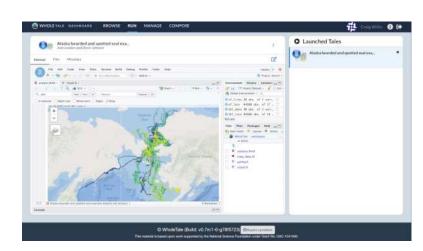


Whole Tale Forecast Demo

Demonstration of a model to predict the movement paths of seals using satellite telemetry data.

Based on analysis and models by:
Josh London and Devin Johnson
NOAA Marine Mammal Laboratory

https://youtu.be/MI5d7r5OtCk











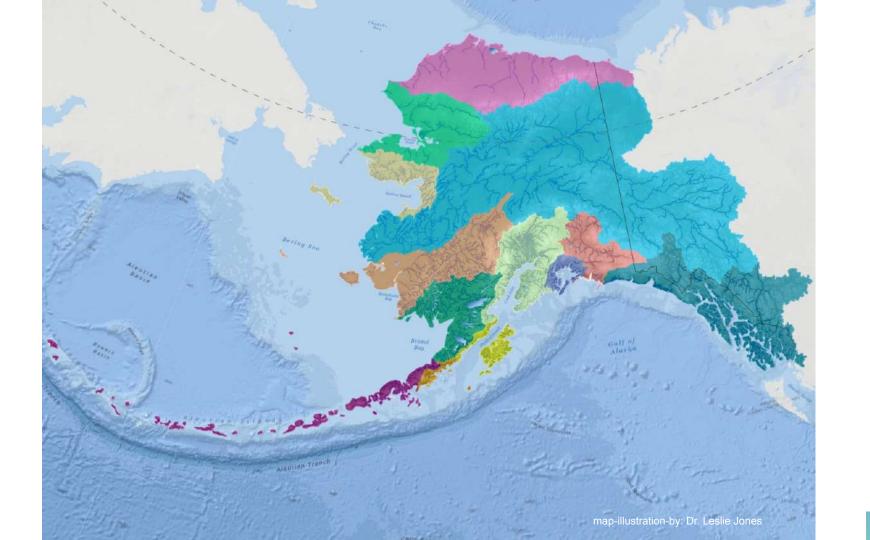
State of Alaska's Salmon and People



8 SASAP working groups

- 1: **Bio-physical State of Knowledge of Salmon Distribution & Habitat**Leads: Peter Westley and Dan Rinella
- 2: **Sociocultural and Economic Dimensions of Salmon Systems**Leads: Courtney Carothers, Jessica Black, Tobias Schworer
- 3: **Governance and Subsistence**Leads: Steve Langdon, Taylor Brelsford, James Fall
- 4: Consistency, Causes, and Consequences of Declining Size and Age of Alaskan Salmon Leads: Eric P. Palkovacs, Peter Westley, Bert Lewis
- 5: **Well-Being and Alaska Salmon Systems**Leads: Rachel Donkersloot, Jessica C. Black, Courtney Carothers
- 6: Interacting Effects of Ocean Climate and At-Sea Competition on Alaskan Salmon Leads: Peter S. Rand, Robert W. Campbell, Kristen B. Gorman
- 7: Using Participatory Modeling to Empower Community Engagement in Salmon Science Leads: Michael L. Jones
- 8: Kenai Lowlands Salmon Research Synthesis and Design Tools for Integrated Watershed Management

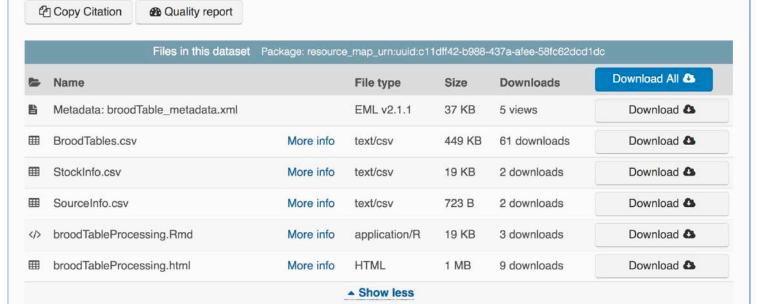
Leads: Coowe Walker, Mark Rains, Ryan King, Charles Simenstad, Dennis Whigham

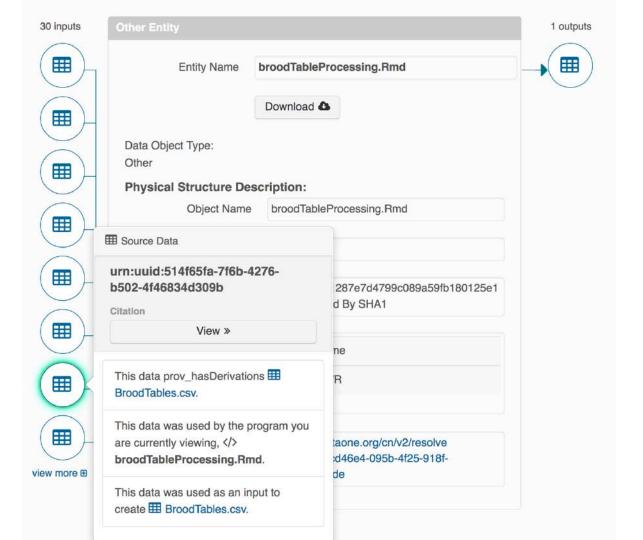


Home / Search / Metadata

Jeanette Clark and Rich Brenner. 2017. Sockeye salmon brood tables, northeastern Pacific, 1922-2016. Knowledge Network for Biocomplexity. urn:uuid:c11dff42-b988-437a-afee-58fc62dcd1dc.



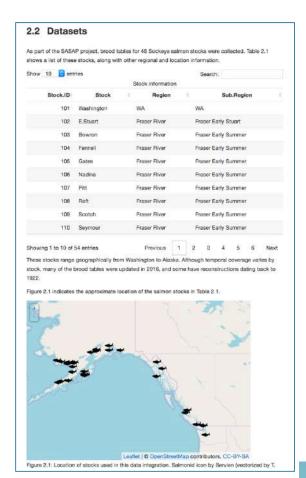




Rmarkdown as Provenance









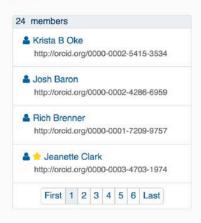


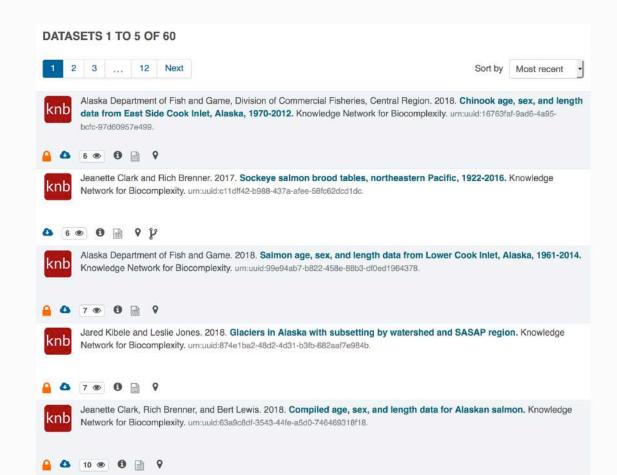
Group Id: SASAP

4 years, 6 months

Contributor since August
4, 2013

- 2 contributions
- 4,862 downloads





Foundational Infrastructure

Providing *findable*, *accessible* data with *interoperable* infrastructure enabling long term data *reuse* for synthesis

