### 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**



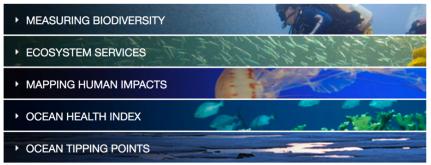
#### Marine Systems



#### Threats and Population Declines



#### Understanding Ocean Health



#### Climate and Ecosystems





### Reproducible Science



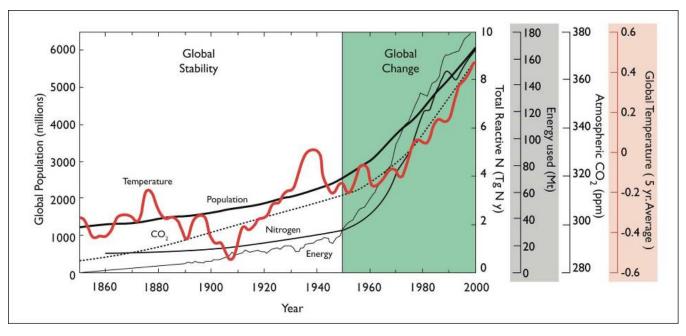
Climate Change Fisheries Sustainabiity Subsistence

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

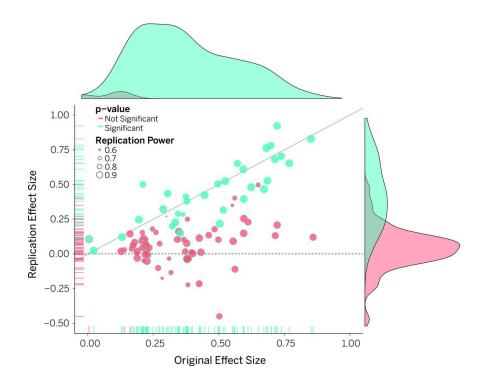
### **Reproducibility Crisis**

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

Ioannidis, 2005

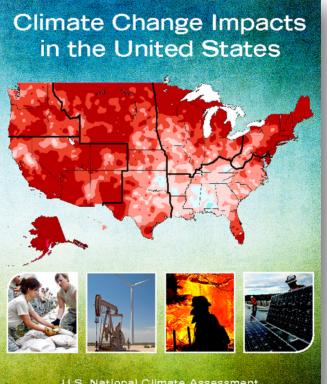
"Most replication effects were smaller than original results"

Open Science Collaboration, 2015



doi:10.1126/science.aac4716

### National Climate Assessment



U.S. National Climate Assessment U.S. Global Change Research Program "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

### Increase **trust in science**

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

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



Practical Reproducibility

Preserve the data

Preserve the software workflow

Document what you did

Describe how to interpret it all



		and the second se	
	KND ABOUT DATA SHARE TOOLS JU	Imp to: DOI or ID Go SIGN IN	and and
× Clear all filters		2	
Search @	DATASETS 1 TO 25 OF 44	de Map »	✓ Limit my search to the map area
Search phrase Q	1 2 Next Sort by Most recent		
My Search sasap X	knb 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.		
Filter by:	<b>△</b> 5 ● <b>1</b> ● <b>2</b>	And the second s	
Data attribute	knb Commercial Fisheries Entry Commission. 2018. Commercial Fisheries Entry Commission Basic Information Table, 1975-2016. Knowledge Network for		10 The second
Data files	Biocomplexity. um:uuid:8f351735-baf9-451a-b821-c1117ebf5a5ej		
Creator			and the second second
Year	Andrew Munro and Eric Volk. 2018. Summary of Pacific Salmon Escapement Goals in Alaska with a Review of Escapements from 2001 to 2009. Knowledge		

Identifier

🚠 Taxon

 $\mathbf{O}$ Location

Network for Biocomplexity. urn:uuid:d62539fd-3025-48d0-a1c3-5a903de1f269. 10 👁 🚺 🗎 💡 8 Alaska Department of Labor and Workforce Development, Research and Analysis knb Section. 2018. Alaskan fishing industry employee counts by month, grouped by region and fish species from 2000-2016. Knowledge Network for

Biocomplexity. urn:uuid:32958097-0ad3-428a-aba9-c37e804be0ef.

₽ 9 8 9 👁 0



Alaska Department of Labor and Workforce Development Research & Analysis Section. 2018. Alaskan fishing industry employee counts by month, subsetted by region and fish species. Knowledge Network for Biocomplexity.

urn:uuid:4bbc9577-e81f-40f4-b4ca-9c740092baba. 9

5 👁 6



Commercial Fisheries Entry Commission. 2018. Commercial Fisheries Entry KND Commission Permit Farnings 1975-2016 Knowledge Network for Biocomplexity

Map data ©2018 Google, INEGI, SK telecom, ZENRIN 500 km

\_\_\_ Terms of Use

AQ SKA

Satellite Terrain



### https://search.dataone.org

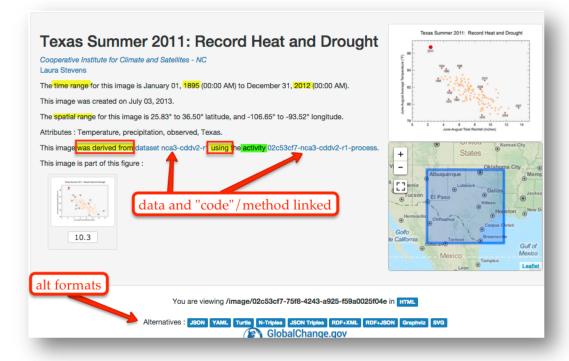




### **Computational Provenance**

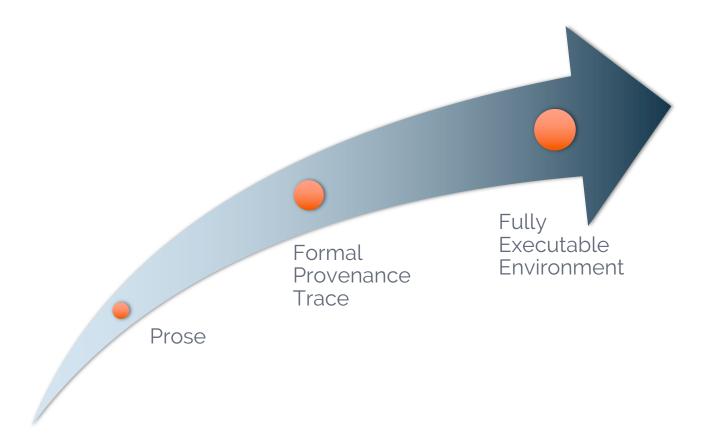
Origin, processing history of data

- 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**

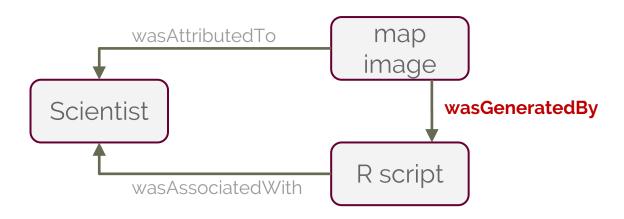
### Provenance for Science Workflows



ProvONE – an extension of W3C PROV

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





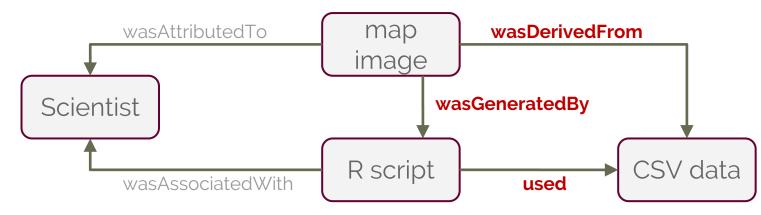
### Provenance for Science Workflows



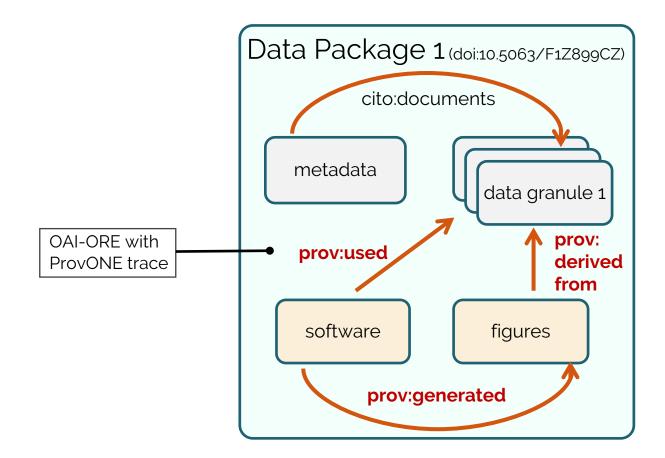
ProvONE – an extension of W3C PROV

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



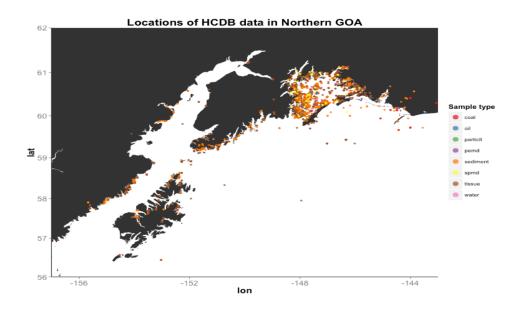


### Data Package with Provenance

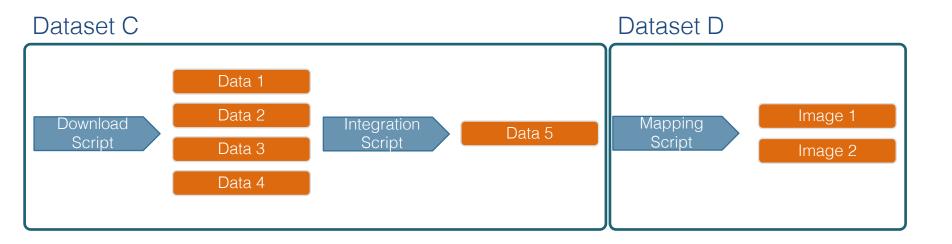


### Hydrocarbon Data Example

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



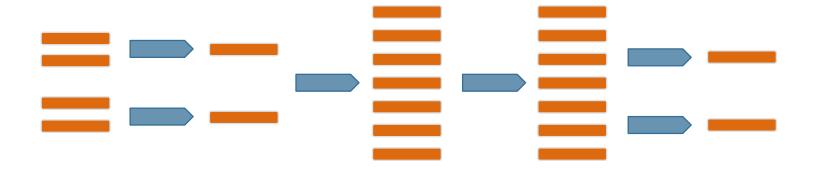
Publishing Data Workflows



Hydrocarbon Data Example

Complex Workflows

Simplified view of complex workflows



### Provenance Display

#### DataONE Search

out N	lews Pa	ticipate	Resources	Educatior	Data						
AONE SEA	RCH: Se	arch	Summary	Jump to:	DOI or ID	Go					Sign in or
< <b>B</b>	ack to searcl	n   S	Search / Metadata	ı							
Dat		urn:uu	Analysis of id:3249ada0-				e Exxon Valdez oil : 71.	spill, Gulf of Ala	aska, 1989 -	2014. Gulf of Al	laska Alaska Ocean Observing System
					Files in t	his dataset	Package: urn:uuid:1d23e15	5-3ef5-47c6-9612-027	:80855e8d		
Þ	Name							File type			Download all 🕰
Ľ	Metadata:	metadat	ta.xml					EML v2.1.1	140 KB	112 views	Download 🕹
⊞	Total_Aror	natic_All	kanes_PWS.csv				More info	text/csv	3 MB	3 downloads	Download 🗳
⊞	Collection	Vethods	CSV				More info	text/csv	793 B	2 downloads	Download 4
_	Non-EVOS	S_SINs.o	CSV				More info	text/csv	3 KB		Download 🕰
⊞											

#### Data Table, Image, and Other Data Details

4 sources	Data Table			2 derivations		
	Entity Name					
		Download 4				
	Description	Combined dataset from PAH, Alkane and Sample tables documenting sa Exxon Valdez oil spill in Prince William Sound, AK	amples collected after the			
	Object Name Total_Aromatic_Alkanes_PWS.csv					
	Online Distribution Info	https://cn.dataone.org/cn/v2/resolve/urn:uuid:44108e76-405d-4d58-l	b1b3-fb4b55e3fff9			
	Size	2801033 byte				
	Text Format	Number of Header Lines	1			
		Record Delimiter	#x0A			
		Attribute Orientation	column			
		Simple Text				
		Field Delimeter	3			
	Number Of Records	12142				

#### Data Table, Image, and Other Data Details

4 sources	Source Pro	gram			2 derivations
	Total_PAH_and_Alkanes_GoA_Hy drocarbons_Clean.R		kanes_PWS.csv		
	View ×	>			
	This program generated the data you are currently viewing, III Total Aromatic Alkanes PWS.csv		om PAH, Alkane and Sample tables documenting sa Il in Prince William Sound, AK	imples collected after the	
			anes_PWS.csv		
	This program used <b>PAH.csv</b> , <b>Sample.csv</b> , <b>Mon-EVOS_SINs.csv</b> and (and 1 more ).		org/cn/v2/resolve/urn:uuid:44108e76-405d-4d58-l	b1b3-fb4b55e3fff9	
	Text Format	Number of Head	er Lines	1	
		Record Delimiter		#x0A	
	Attribute Orientation		tion	column	
				3	
	Number Of Records	12142			

### Web Provenance Editor

### Deployed by Arctic Data Center

	NSF Arctic Data Center	
ARCTIC Data Center	Data Support About Submit	Data Christopher Jones
Data Table, Image, and Other Data De	tails	
0 sources Data Table		0 derivations
Add Entity Name	Total_Aromatic_Alkanes_PWS.csv	
	Download	
Description	Combined dataset from PAH, Alkane and Sample tables documenting samples collected after the Exxon Valdez oil spill in Prince William Sound, AK	
Object Name	Total_Aromatic_Alkanes_PWS.csv	
Online Distribution Info	https://cn- stage.test.dataone.org/cn/v2/resolve/urn:uuid:df984766-dd89- 4e57-b97e-350506d7007e	
Size	2801033 byte	
Text Format	Number of Header Lines 1	
	Record Delimiter #x0A	





### **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

#### Derived image

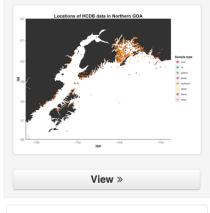
Map of sampling locations in the Northern Gulf of Alaska

Citation

Mark Carls. 2015. Hydrocarbon

database, Gulf of Alaska. MN

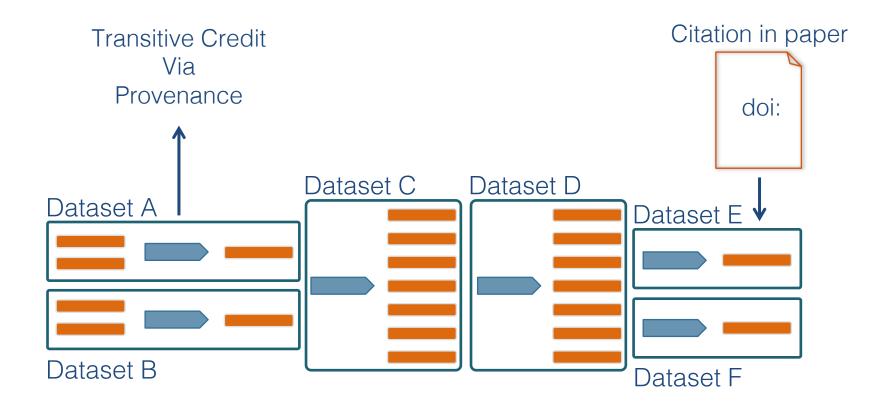
Demo 2. urn:uuid:bf71c38b-22b2-46 9e-8983-734ec0ab19cb.



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

This image was derived from **H** Total\_Aromatic\_Alkanes\_PWS.csv .

### Citing multi-generational workflows



### Evolution of the Living Paper







### Scholarly Publications

1 <sup>st</sup> Gen	Prose		
2 <sup>nd</sup> Gen	Prose	+ Data	
3 <sup>rd</sup> 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

#### Authors and affiliations

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







Follow

## 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

🖿 data

replicationDemos
 help
 Meta

🛅 demo

html

Rdata.rdx

replicationDemos.rdb

replicationDemos.rdx replicationDemos

Rdata.rdb

Rdata.rds

INDEX



DESCRIPTION



## **Parsing Reproducibility**

### Empirical Reproducibility:

• traditional empirical experiments, e.g. at the bench/lab

### Statistical Reproducibility:

• statistical methodology used permits generalizability of data inferences

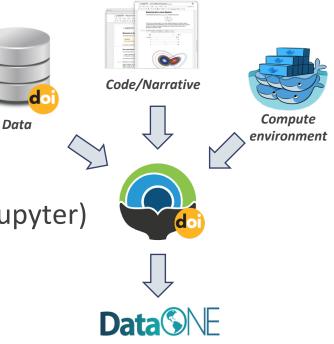
### • **Computational** Reproducibility:

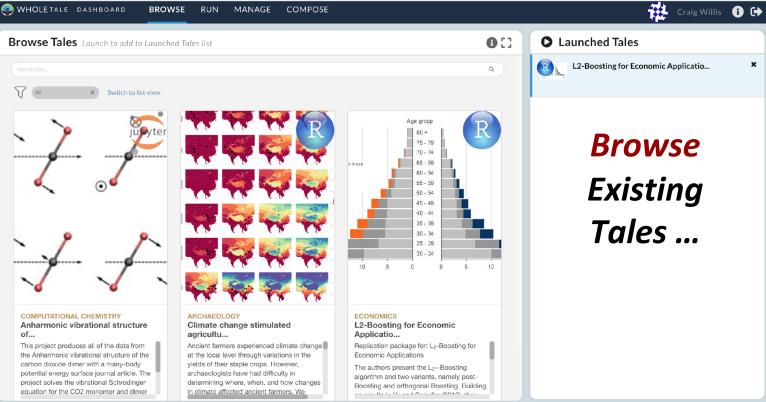
• transparency of computational steps that produce scientific findings



# 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





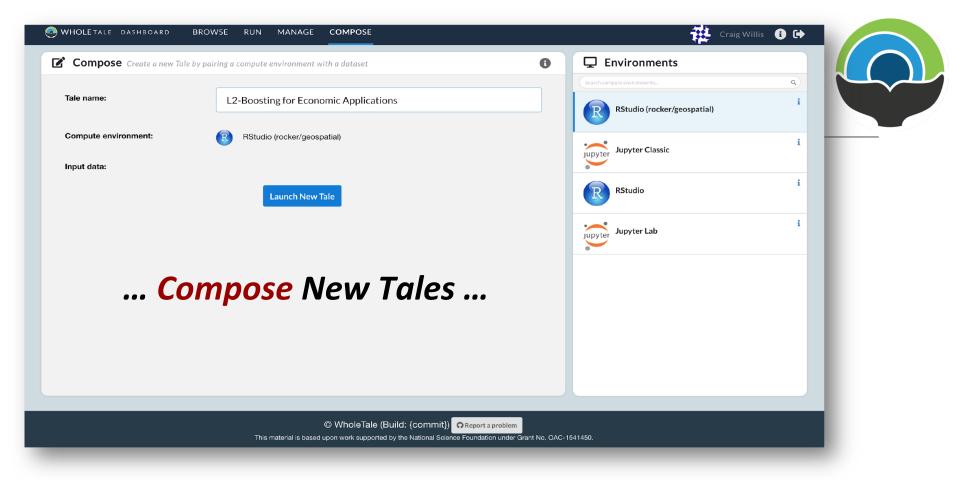


×

Existing Tales ...

© WholeTale (Build: {commit})

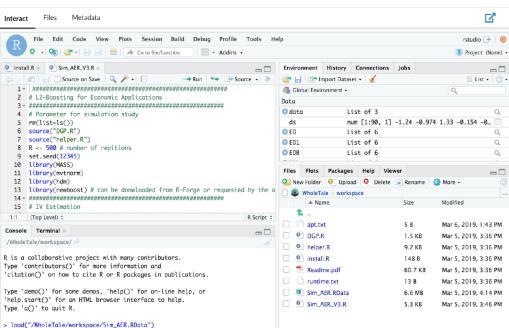
This material is based upon work supported by the National Science Foundation under Grant No. OAC-1541450.

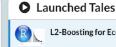


L2-Boosting for Economic Applicatio... Ye Luo and Martin Spindler

R

>





:

L2-Boosting for Economic Applicatio...

- ti

Craig Willis 🚯 🛟

×



... Run & Interact with Tales

...

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

#### Data Search - About User Guide Support Sign Up Log In Resources Education Data DATAONE SEARCH: Search Summary Jump to: DOI or ID Go Sian in or Sian up AMERICAN JOURNAL of POLITICAL SCIENCE Search / Metadata tical Science (AJPS) Dataverse (Midwest Political Science Association) ains org Daniel White and Lilian Alessa. Humans and Hydrology at High Latitudes: Water Use Information. Arctic Journal of Political Science (AJPS) Dataverse > Replication Data for: Greater Expectations: A Field Experiment to Improve Accountability in Mali Data Center, doi:10.5065/D6862DM8 Contact Et Share Choose an analysis environment to ctively explore this datase online using Whole Tale ata for: Greater Expectations: A Field Experiment to Improve Accountability in Mali **55** Citations 0 Downloads 183 Views 72 Copy Citation III Analyze plication Data for: Greater Expectations: A Field Experiment to Improve Accountability in Explore - Explore -RStudio VDVN/29040, Harvard Dataverse, V3, UNF:6:CCpgASJQMfVBn0+Hn/PM1Q== [fileUNF] Jupyter Notebook Learn about Data Citation Standards. Files in this dataset Package: resource\_map\_doi:10.5065/D6862DM8 Analyze in WT Download All 🕰 I aroue that if citizens systematically underestimate what their covernment can and should do for them, then they will hold Download 🕰 politicians to a lower standard and sanction poor performers less often. A field experiment across 95 localities in Mali in which Metadata: science metadata.xml EML v2.1.1 8 KB 65 views randomly assigned localities receive a civics course identifies the effect of raising voter expectations of government on their willingness to hold leaders accountable. The course provides information about local government capacity and responsibility as Download A m estimated\_use\_of\_water\_in\_US\_2000.pdf PDF 6 MB 6 downloads well as how local politicians perform relative to others, effectively raising voter expectations of what local governments can and should do. Survey experiments among individuals in treated and control communities (N=5,560) suggest that people in treated villages are indeed more likely to sanction poor performers and vote based on performance more often. A behavioral outcome -" Download 🕰 PDF m estimated\_use\_of\_water\_in\_US\_2005.pdf 5 MB 5 downloads the likelihood that villagers challenge local leaders at a town hall meeting - adds external validity to survey findings. Download 🕰 Social Sciences first\_nations\_canada\_water\_and\_wastewater\_systems.pdf PDF 365 KB 4 downloads Government accountability, Voting behavior, Field experiments > Show 13 more items in this data set Gottlieb, Jessica. 2016. "Greater Expectations: A Field Experiment to Improve Accountability in Mali." American Journal of Political Science 60 (1): 143-157. doi: 10.1111/ajps.12186 General Identifier doi:10.5065/D6862DM8 Q, Find id%3Ddoi%3A10.7910%2FDVN%2F29040&name=Replication Data for%3A Greater Expectations%3A A Field Experiment to Im

... 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 ()
    environment.json ()
    LICENSE ()
    README.md ()
    metadata.xml ()

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.



-



## ... Publish Data, Code, and Environment

 Enables full circle reproducibility to DataONE

repositories that accept API deposits

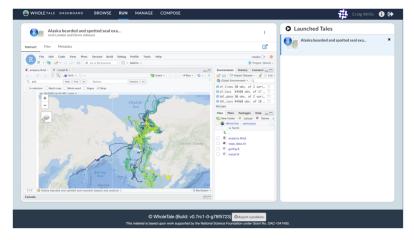


# Whole Tale Forecast Demo

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

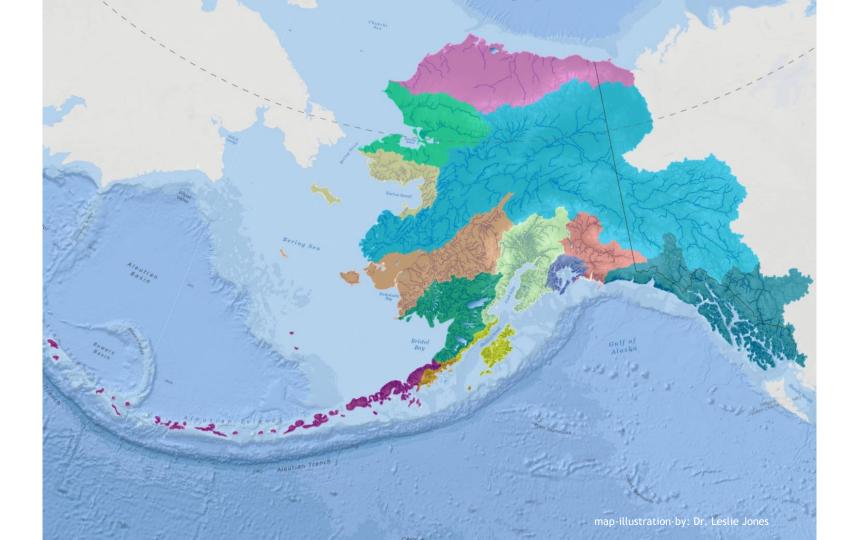
4: Consistency, Causes, and Consequences of Declining Size and Age of Alaskan Salmon Leads: Eric P. Palkovacs, Peter Westley, Bert Lewis

#### 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



	knb	ABOUT	DATA	SHARE	TOOLS	Jump to:	DOI or ID Go	SIGN IN
1		1	1 Store La	a de la cal	- Color	1		
н	ome / Search /	Metadata						
2	notto Clark a	and Rich Brei	oper 2017	Sockeye salr	non brood tabl	les northe	astern Pacific	
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.								
KND								
_								
æ	] Copy Citation	Quality	report					
æ	] Copy Citation			Package: resource	e_map_urn:uuid:c1	1dff42-b988-	437a-afee-58fc62dc	d1dc
2	Copy Citation			Package: resource	e_map_urn:uuid:c1 File type	1dff42-b988- <b>Size</b>	437a-afee-58fc62dc Downloads	d1dc Download All 🕭
2	Name		nis dataset F	Package: resource		_		
•	Name	Files in th	nis dataset F	Package: resource More info	File type	Size	Downloads	Download All 🕭
•	Name Metadata: bro	Files in th podTable_metac	nis dataset F		File type EML v2.1.1	Size 37 KB	Downloads 5 views	Download All 💿 Download 🕰
•	Name Metadata: bro BroodTables.e	Files in the podTable_metac	nis dataset F	More info	File type EML v2.1.1 text/csv	<b>Size</b> 37 KB 449 KB	Downloads 5 views 61 downloads	Download All  Download  Download  Download  Download
	Name Metadata: bro BroodTables.o StockInfo.csv SourceInfo.cs	Files in the podTable_metac	nis dataset F	More info More info	File type EML v2.1.1 text/csv text/csv	<b>Size</b> 37 KB 449 KB 19 KB	Downloads5 views61 downloads2 downloads	Download All  Download  Do

30 inputs	Other Entity			1 outputs
	Entity Name	broodTableF	Processing.Rmd	
		Download	2	
	Data Object Type: Other			
	Physical Structure De	scription:		
	Object Name	broodTable	Processing.Rmd	
	Bource Data			
	urn:uuid:514f65fa-7f6b-4	276-		
	b502-4f46834d309b Citation		287e7d4799c089a59fb180125e1 d By SHA1	
	View »			
			ne	
	This data prov_hasDerivatio BroodTables.csv.	ns 🎫	R	
	This data was used by the p	rogram you		
view more 🕀	are currently viewing,  broodTableProcessing.Rm	ıd.	taone.org/cn/v2/resolve :d46e4-095b-4f25-918f- de	
	This data was used as an in create III BroodTables.csv.	put to		

### Python, Jupyter and Rmarkdown as Provenance



#### 2.2 Datasets

As part of the SASAP project, brood tables for 48 Sockeye salmon stocks were collected. Table 2.1 shows a list of these stocks, along with other regional and location information.

Show 10 ᅌ entr	ies		Search:		
		Stock information			
Stock.ID	Stock 0	Region 0	Sub.Region		
101	Washington	WA	WA		
102	E.Stuart	Fraser River	Fraser Early Stuart		
103	Bowron	Fraser River	Fraser Early Summer		
104	Fennell	Fraser River	Fraser Early Summer		
105	Gates	Fraser River	Fraser Early Summer		
106	Nadina	Fraser River	Fraser Early Summer		
107	Pitt	Fraser River	Fraser Early Summer		
108	Raft	Fraser River	Fraser Early Summer		
109	Scotch	Fraser River	Fraser Early Summer		
110	Seymour	Fraser River	Fraser Early Summer		

Showing 1 to 10 of 54 entries

Previous These stocks range geographically from Washington to Alaska. Although temporal coverage varies by stock, many of the brood tables were updated in 2016, and some have reconstructions dating back to 1922.

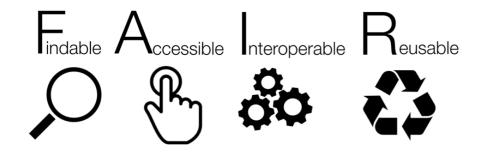
Figure 2.1 indicates the approximate location of the salmon stocks in Table 2.1.



Figure 2.1: Location of stocks used in this data integration. Salmonid icon by Servien (vectorized by T.

Foundational Infrastructure

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



https://www.force11.org/fairprinciples