

Using FAIR principles to improve the usability of a food- energy-water system simulation model

Andrew Hamilton
2021 FAIR Workshop
June 2, 2021

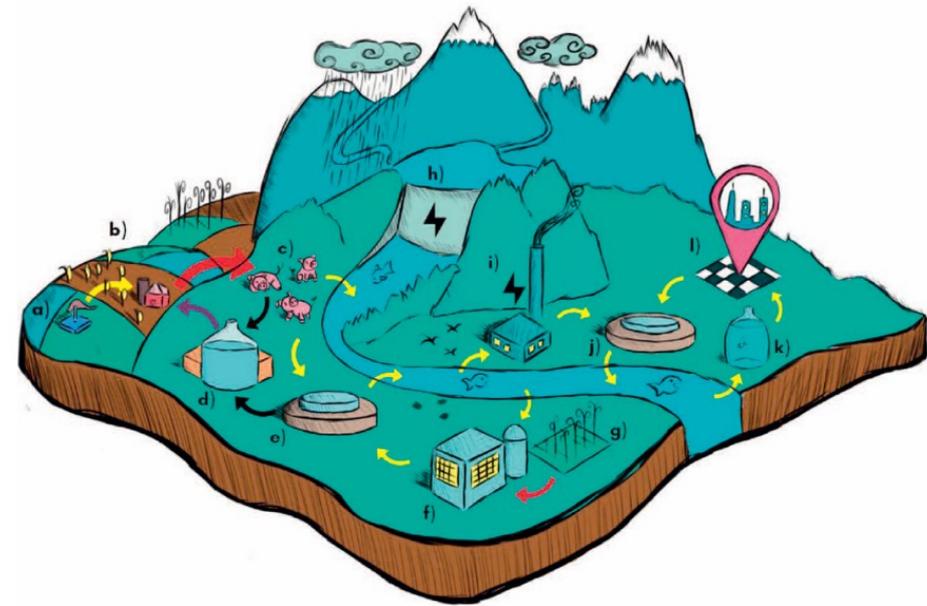
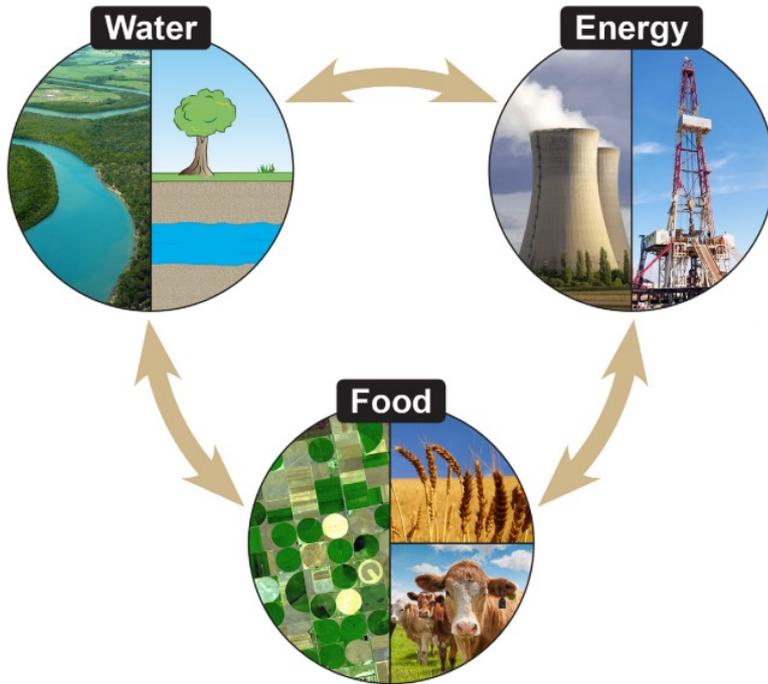


THE UNIVERSITY
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at CHAPEL HILL

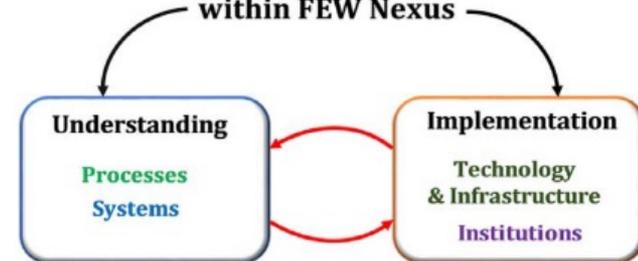


andrew.hamilton@unc.edu

Food-Energy-Water Nexus



Water Resources Research within FEW Nexus

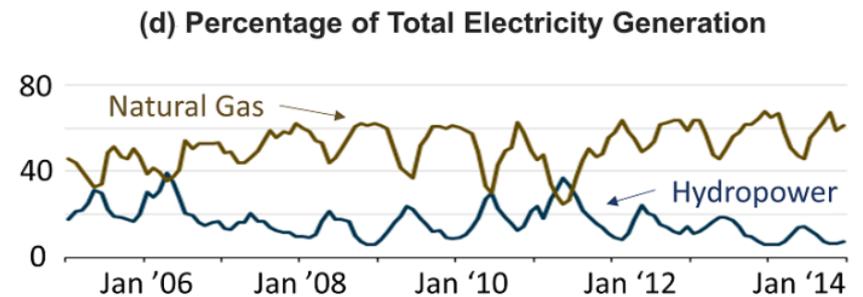
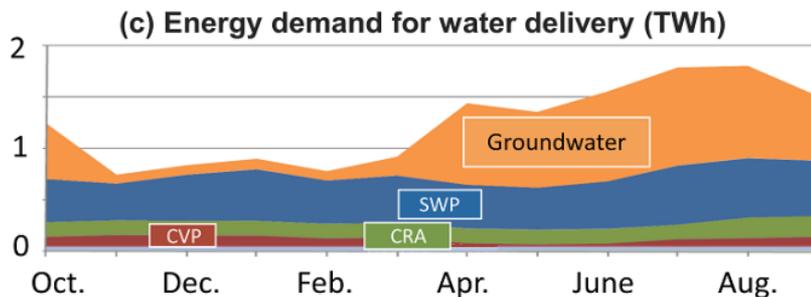
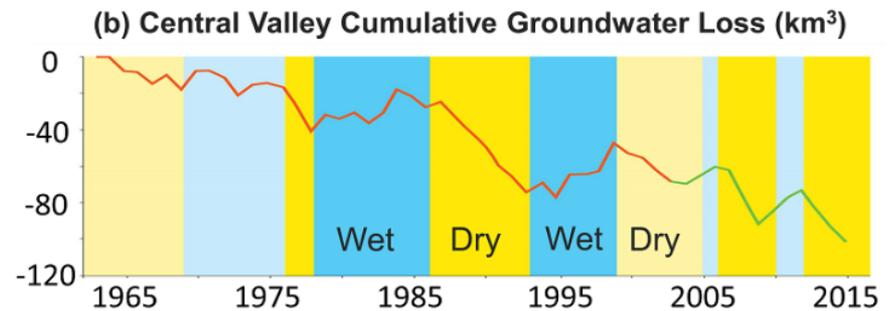
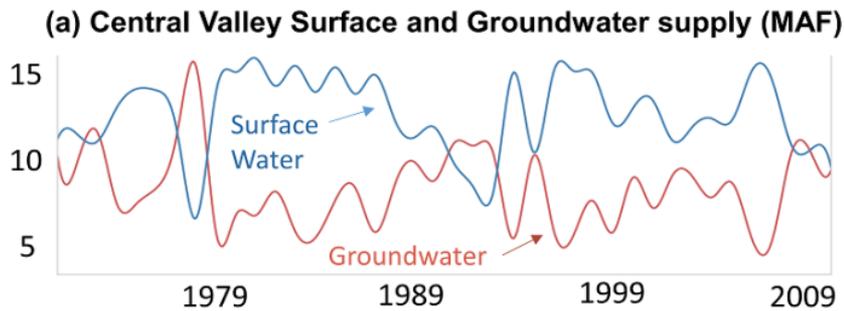


Scanlon et al. (2017). The food-energy-water nexus: Transforming science for society. *Water Resources Research*, 53(5): 3550-3556.

Cai et al. (2018). Understanding and managing the food-energy-water nexus – opportunities for water resources research. *Advances in Water Resources*, 111: 259-273.

Food-Energy-Water Nexus

California as “laboratory” for exploring connections & implications for management



Drought in California

Search **The Guardian** US edition

California is on the brink of drought - again. Is it ready?

Maanvi Singh
@maanvissingh
Tue 6 Apr 2021 06.00 EDT

 **Gavin Newsom** ✓
@GavinNewsom

5:01 PM · Apr 21, 2021

Where I'm standing I should be 40 ft under the water of Lake Mendocino.

Instead--I'm on dry, cracked earth. That's climate change.

Today I declared a drought conditions state of emergency in Mendocino & Sonoma to immediately increase drought resilience. [kcra.com/article/gov-ne...](https://www.kcra.com/article/gov-ne...)



Los Angeles Times

By LOUIS SAHAGÚN
APRIL 26, 2021 UPDATED 10 AM PT

Wells dry up, crops imperiled, farm workers in limbo as California drought grips San Joaquin Valley

≡ **CAL MATTERS**

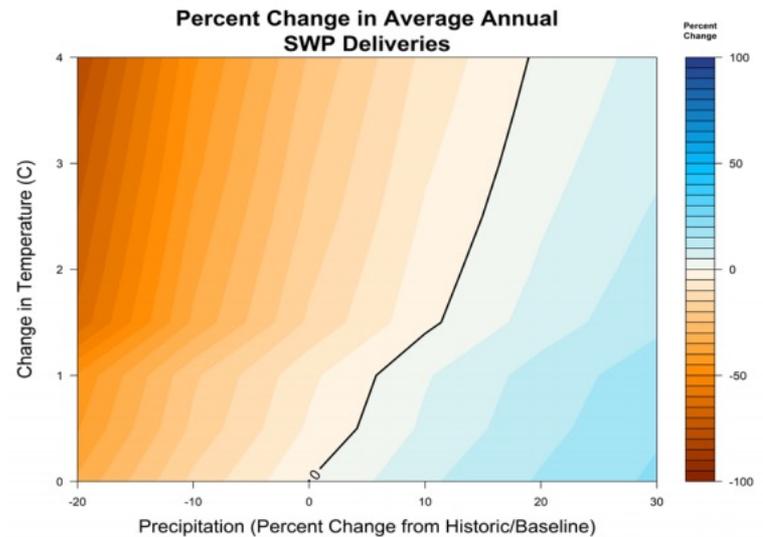
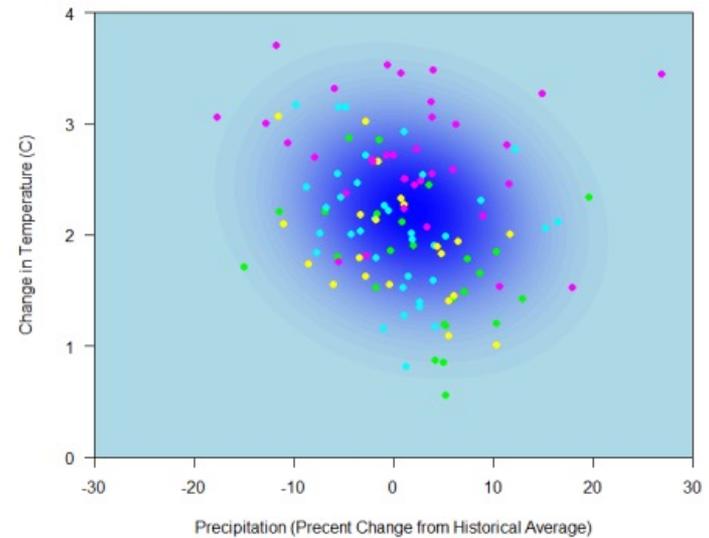
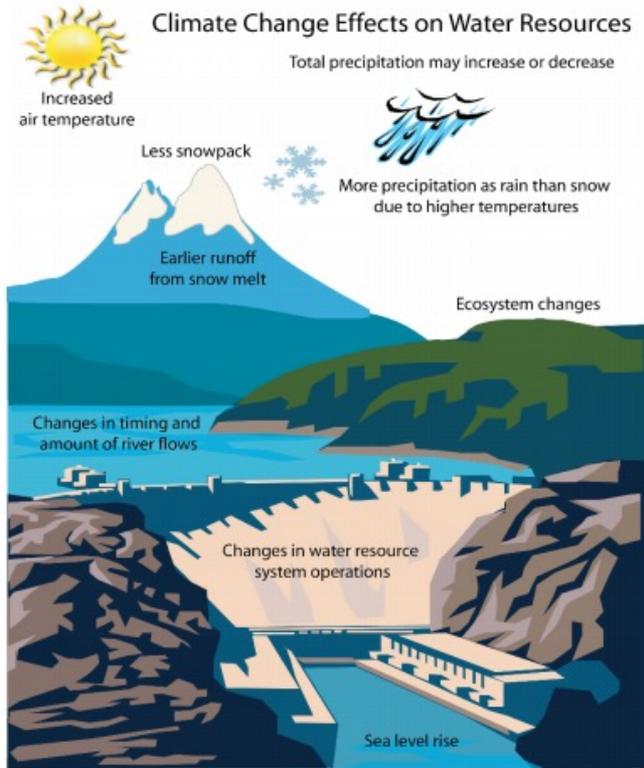
DONATE SUBSCRIBE ABOUT 🔍

As drought hits California, long-term issues loom

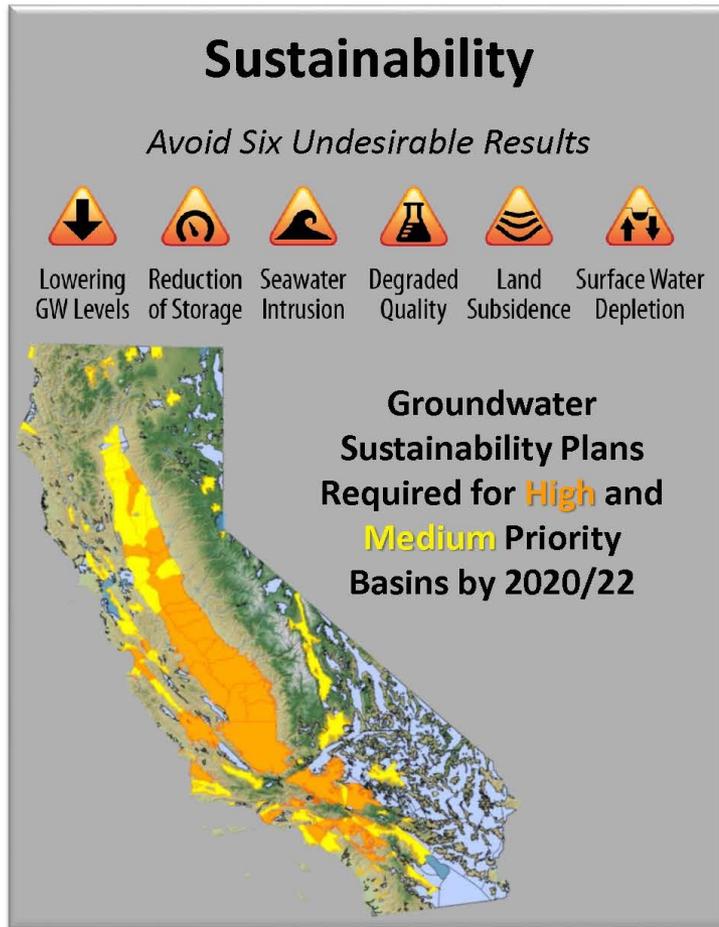
 BY DAN WALTERS
APRIL 25, 2021

Climate change and water resources



Environmental regulation

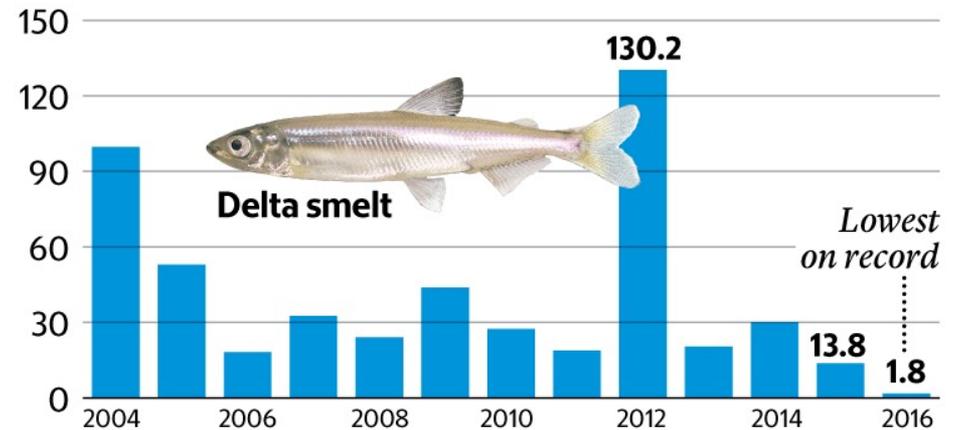


<https://mavensnotebook.com/2017/08/31/state-water-board-update-on-sigma-implementation/>

Delta smelt abundance

Scientists use trawl nets to survey smelt populations at many Delta locations. They report the results as an index of the number of fish relative to the volume of water sampled.

Spring adult index

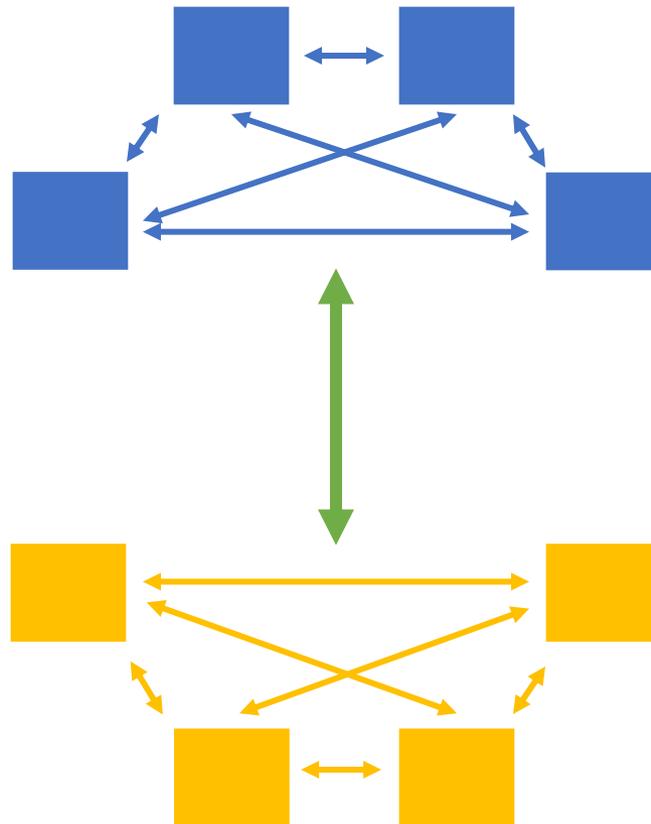


Sources: California Department of Fish and Wildlife

The Sacramento Bee

The Sacramento Bee.

Actions of other water users



Irrigation districts

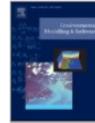
Urban utilities

California Food-Energy-Water System (CALFEWS)



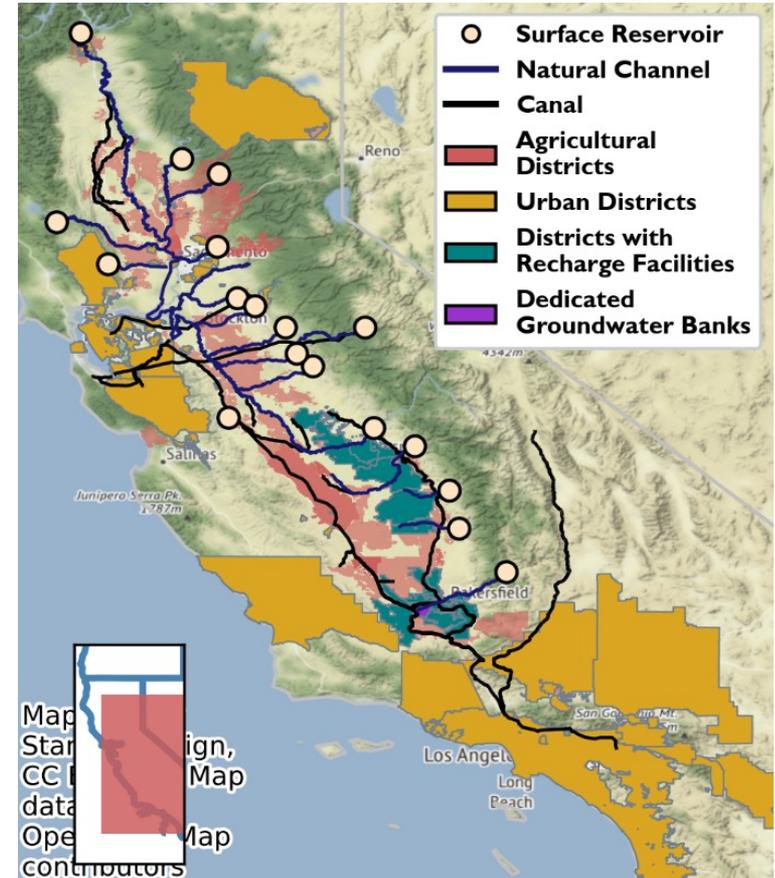
Environmental Modelling & Software

Volume 141, July 2021, 105052



California's food-energy-water system: An open source simulation model of adaptive surface and groundwater management in the Central Valley

Harrison B. Zeff^a, Andrew L. Hamilton^a, Keyvan Malek^b, Jonathan D. Herman^c, Jonathan S. Cohen^c, Josue Medellin-Azuara^d, Patrick M. Reed^b, Gregory W. Characklis^e



GitHub repository interface for hbz5000 / CALFEWS. The interface includes a search bar, navigation links for Pull requests, Issues, Marketplace, and Explore, and a list of repository tabs: Code, Issues, Pull requests, Actions, Projects, Wiki, Security, and Insights. The main branch is 'main' with 2 branches and 1 tag. Buttons for 'Go to file', 'Add file', and 'Code' are visible.

<https://github.com/hbz5000/CALFEWS>

FACT Fellowship

Project pt. I: Making CALFEWS model more FAIR

- Goal: Make it easier for other academics & government employees to adopt CALFEWS for research &/or planning purposes
- Improve README & documentation of code organization on GitHub
- Improve documentation of input data sources
- Create Jupyter notebooks to introduce user to running code and to reproduce paper figures
- Create code-free GUI on MyGeoHub for running scenarios & visualizing results

GUI for CALFEWS

The screenshot shows the MyGeoHub website interface. At the top, the MyGeoHub logo is on the left, and navigation links for RESEARCH, RESOURCES, COMMUNITY, TEACHING, SUPPORT, and ABOUT are on the right. A user profile for Andrew L Hamilton is also visible. Below the navigation bar, a breadcrumb trail reads: Home / Tool Forge / Tools / Graphical User Interface for the California Food-Energy-Water System (CALFEWS) simulation model / About. A search bar is located on the right side of this section.

Graphical User Interface for the California Food-Energy-Water System (CALFEWS) simulation model

By Andrew L Hamilton, Harrison Zeff, Keyvan Malek, Jonathan Herman, Jonathan Cohen, Josue Medellin-Azuara, Patrick M. Reed, Gregory W. Characklis

Graphical User Interface for the California Food-Energy-Water System (CALFEWS) simulation model

[About](#) [Usage](#) [Versions](#) [Reviews](#) [Questions](#) [Wishlist](#) [Supporting Docs](#)

Category: [Tools](#) Published on: 04 Feb 2021

Abstract

This tool provides a graphical user interface for the [California Food-Energy-Water System \(CALFEWS\)](#), an open-sourced, Python-based model for simulating the integrated, multi-sector dynamics of water supply in the Central Valley of California. CALFEWS captures system dynamics across multiple scales, from coordinated management of inter-basin water supply projects at the state and regional scale, to agent-based representation of conjunctive surface water and groundwater supplies at the scale of irrigation and water storage districts. This user interface can be used to simulate operations under different hydrologic conditions and visualize the results using the interactive plotting features.

Credits

A.L.H. is grateful for guidance from Venkatesh Merwade, Carol Song, Matthew Huber, Lan Zhao, and I Luk Kim. This graphical user interface was developed under the FAIR Cyber Training Fellowship program at Purdue University (NSF Award #1829764). Development of the CALFEWS simulation model is supported under an INFEWS/T2 grant (Award #1639268)

Launch Tool

Version 1.0 - published on 04 Feb 2021
doi:10.21981/AH5Y-G419 [cite this](#)
Open source: [license](#) | [download](#)

[View All Supporting Documents](#)

1 users, detailed usage

Share: [f](#) [t](#) [l](#) [v](#)

0 review(s)

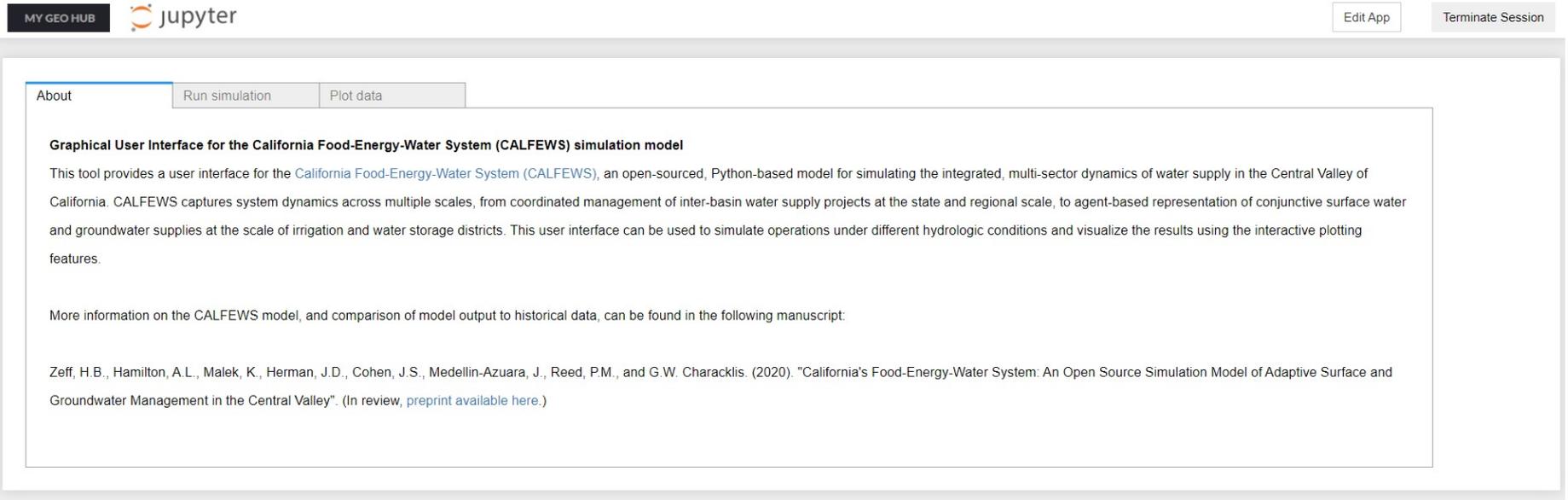
0 questions (Ask a question)

0 wish(es) (New Wish)

Watch resource

When watching a resource, you will be notified of changes made. You may stop watching at any time.

GUI for CALFEWS



The screenshot shows a Jupyter interface with a dark header bar containing "MY GEO HUB" and the "jupyter" logo. On the right side of the header are two buttons: "Edit App" and "Terminate Session". Below the header is a light gray content area with a navigation bar at the top left containing "About", "Run simulation", and "Plot data". The "About" tab is active, displaying the following text:

Graphical User Interface for the California Food-Energy-Water System (CALFEWS) simulation model

This tool provides a user interface for the [California Food-Energy-Water System \(CALFEWS\)](#), an open-sourced, Python-based model for simulating the integrated, multi-sector dynamics of water supply in the Central Valley of California. CALFEWS captures system dynamics across multiple scales, from coordinated management of inter-basin water supply projects at the state and regional scale, to agent-based representation of conjunctive surface water and groundwater supplies at the scale of irrigation and water storage districts. This user interface can be used to simulate operations under different hydrologic conditions and visualize the results using the interactive plotting features.

More information on the CALFEWS model, and comparison of model output to historical data, can be found in the following manuscript:

Zeff, H.B., Hamilton, A.L., Malek, K., Herman, J.D., Cohen, J.S., Medellin-Azuara, J., Reed, P.M., and G.W. Characklis. (2020). "California's Food-Energy-Water System: An Open Source Simulation Model of Adaptive Surface and Groundwater Management in the Central Valley". (In review, [preprint available here.](#))

GUI for CALFEWS

MY GEO HUB



Edit App

Tr

About Run simulation Plot data

Select inflow scenario

Historical validation 1997-2016
Historical reconstruction 1906-2016
2-year example
22-year synthetic
WRF 2007-2017

Folder name to save results (no spaces)

2-year_example

Click to begin

Start

Progress

Inflow scenario	Description	Est. runtime (mins.)
Historical validation 1997-2016	20-year simulation using historical data and infrastructure (see Zeff et al., 2020, https://engrxiv.org/sqr7e)	11
Historical reconstruction 1906-2016	111-year simulation using statistically-reconstructed data and 2017 infrastructure (see Zeff et al., 2020, https://engrxiv.org/sqr7e)	56
2-year example	2-year example simulation, with wet year (1997) followed by dry year (2014)	2
22-year synthetic	22-year synthetic dataset using the CAPOW stochastic engine (see Su et al., 2020, https://doi.org/10.1016/j.envsoft.2020.104667)	12

GUI for CALFEWS

MY GEO HUB



Edit App

About Run simulation Plot data

Select inflow scenario

- Historical validation 1997-2016
- Historical reconstruction 1906-2016
- 2-year example
- 22-year synthetic
- WRF 2007-2017

Folder name to save results (no spaces)

2-year_example

Click to begin

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Inflow scenario	Description	Est. runtime (mins.)
Historical validation 1997-2016	20-year simulation using historical data and infrastructure (see Zeff et al., 2020, https://engrxiv.org/sqr7e)	11
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2-year example	2-year example simulation, with wet year (1997) followed by dry year (2014)	2
22-year synthetic	22-year synthetic dataset using the CAPOW stochastic engine (see Su et al., 2020,	12

```
#####
Begin initialization...
Initialization complete, 0:00:52.893097
Begin simulation, 0:00:52.893791
temp/sim/2-year_example
Year 1.0 , 0:01:28.627244
Year 2.0 , 0:01:56.171116
Simulation complete, 0:01:58.904889
#####
Copying data to ~/data/CALFEWS/2-year_example
Finished! Proceed to "Plot data" tab.
```

GUI for CALFEWS

The screenshot shows the user interface of the CALFEWS application. At the top left, there is a dark grey bar with the text "MY GEO HUB" and the Jupyter logo. To the right of this bar is a button labeled "Edit App". Below the top bar is a horizontal navigation menu with three tabs: "About", "Run simulation", and "Plot data". The "Plot data" tab is currently selected and highlighted with a blue border. The main content area of the application is titled "Select dataset" and contains a text input field with the following text: "2-year_example" and "CanESM2_RCP_4.5_1951-2100".

GUI for CALFEWS

About Run simulation **Plot data**

Select dataset

2-year_example
CanESM2_RCP_4.5_1951-2100

Loading data from ~/data/CALFEWS/CanESM2_RCP_4.5_1951-2100/

Select subset of data for figures

Reservoir ▾

Choose attribute, compare reservoirs ▾

Storage (tAF) ▾

Shasta Lake
Lake Oroville
New Bullards Bar Reservoir
Folsom Lake
New Melones Lake

GUI for CALFEWS

Figure 1: Full time series (click and drag to select zoom region for Figure 2)

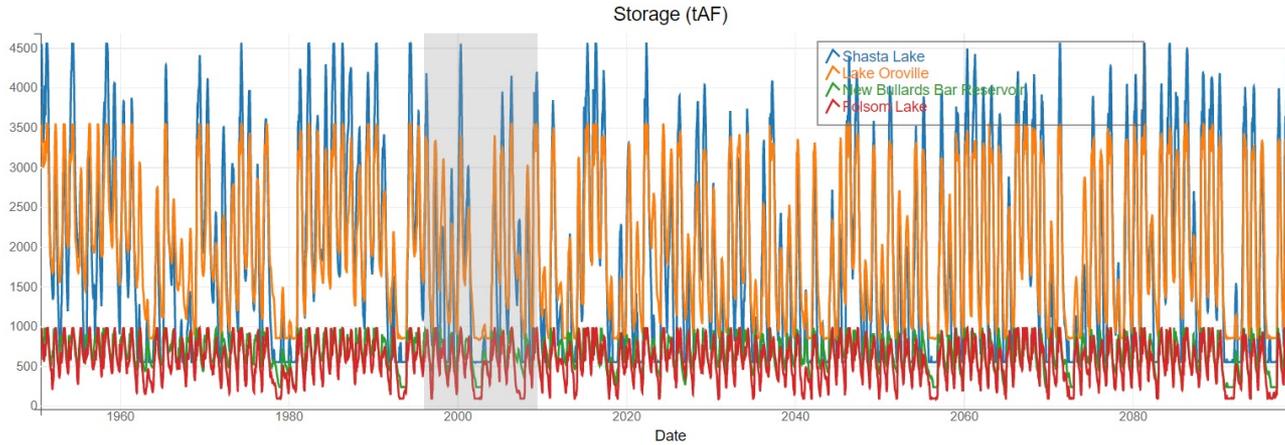
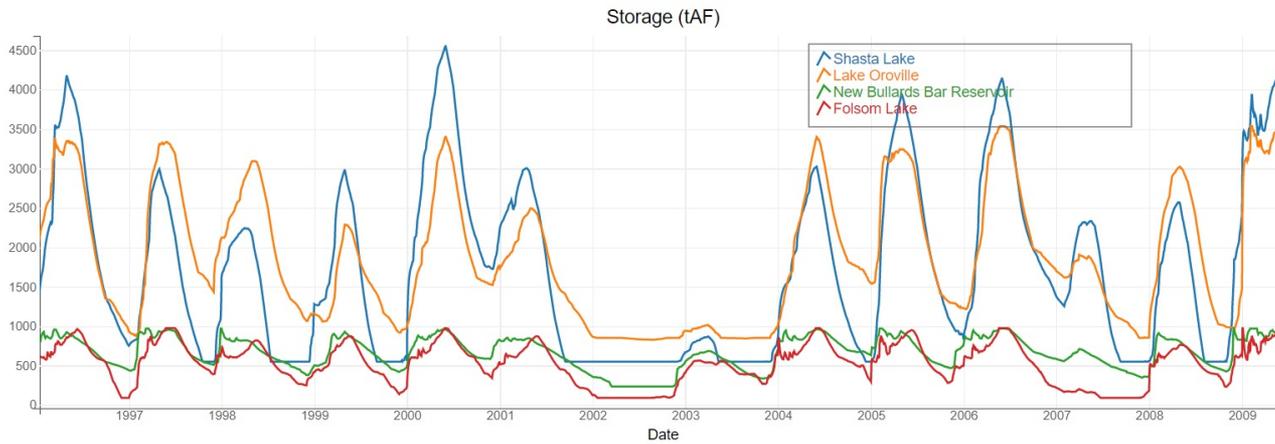


Figure 2: Zoomed in time series



Download full dataset or subset of data

(buttons will create link below plots)

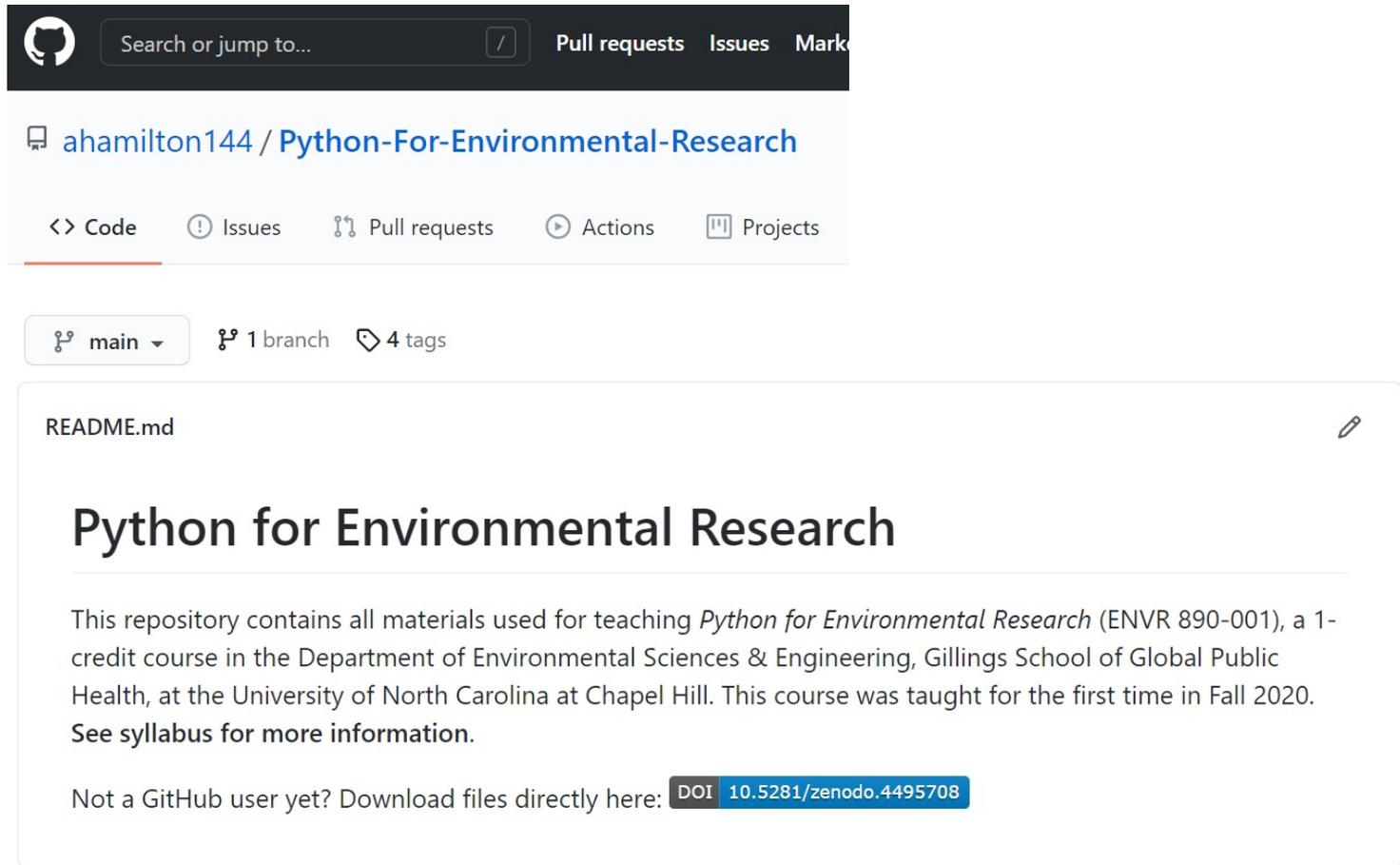
Full dataset

Subsetting dataset



FACT Fellowship

Project pt. 2: Integrate FAIR principles into course



The screenshot shows the GitHub interface for the repository 'ahamilton144 / Python-For-Environmental-Research'. The repository is on the 'main' branch, has 1 branch and 4 tags. The README.md file is displayed, featuring the title 'Python for Environmental Research' and a description: 'This repository contains all materials used for teaching *Python for Environmental Research* (ENVR 890-001), a 1-credit course in the Department of Environmental Sciences & Engineering, Gillings School of Global Public Health, at the University of North Carolina at Chapel Hill. This course was taught for the first time in Fall 2020. See syllabus for more information.' A link is provided for non-GitHub users to download files directly: DOI 10.5281/zenodo.4495708.

Python for Environmental Research course

The screenshot shows the MyGeoHub interface for the 'Python for Environmental Research' course. The header includes the MyGeoHub logo, navigation links (RESEARCH, RESOURCES, COMMUNITY, TEACHING, SUPPORT, ABOUT), and a user profile for Andrew L. Hamilton. The breadcrumb trail is Home / Courses / Python for Environmental Research / Overview. The course title is 'Python for Environmental Research', with a short description: 'Teaching materials for an introduction to using Python for environmental research.' A breadcrumb trail for categories is shown: Environmental Science > Jupyter Notebooks > Public Health > python > teaching > Water Resources. The course is brought to you by 'Cyber Training for FAIR Science'. The main content area has tabs for Overview, Reviews, Offerings, and an Add page button. The long description states: 'NOTE: Still in development. This course provides lectures and homework exercises (as a collection of Jupyter Notebooks) designed to introduce students to computer programming in Python through the lens of environmental research. Students will develop a working knowledge of the Python programming language and learn how to formulate research questions as computer code. They will learn about a variety of Python-based packages and techniques that can be used to build models, analyze data, and create visualizations for research in environmental sciences, engineering, and health. We will take an applications-based approach, with new techniques applied to examples such as air quality monitoring, reservoir management, disease spread, power markets, and environmental justice.' On the right sidebar, there are sections for 'Time & Effort' (Self Paced), 'Instructors/Managers', and 'About the Instructor' (Andrew L. Hamilton, University of North Carolina at Chapel Hill). A note indicates the instructor has yet to write their bio.

Python for Environmental Research course

- Progress
- Pages
- Announcements
- Dashboard
- Notes
- Discussions
- Getting Started

- Introduction to Jupyter & Python
- Basic data structures
- Conditions, functions, & loops
- Advanced data structures
- Systems of equations & optimization
- Data, visualization, & regression
- Simulation, Monte Carlo, & time series
- Geospatial analysis

Python for Environmental Research course

<input type="radio"/>	Systems of equations & optimization	▼
Lectures	<input type="radio"/>	Notes: Systems of equations & optimization
		Notes: Systems of equations & optimization
		Lec5_SystemsEquations.ipynb
Activities	<input type="radio"/>	Homework: Systems of equations & optimization
		Homework: Systems of equations & optimization
		HW5_SystemsEquations.ipynb

Python for Environmental Research course

Slide Type Slide ▾

Lecture 5: Systems of equations & optimization

ENVR 890-001: Python for Environmental Research, Fall 2020

September 18, 2020

By Andrew Hamilton, some material adapted from Greg Characklis, David Gorelick, and H.B. Zeff.

Slide Type Fragment ▾

Summary

Now that we have covered the basics of Python programming (e.g., variable types, data structures, if statements, loops, functions), we can move on to **solving problems** in environmental science, engineering, and public health. The first type of problem we will solve will be **systems of equations and optimization**.

This will involve a bit of math, but we will try to focus on the programming elements.

Slide Type Slide ▾

Linear system of equations

Systems of equations appear in many different fields of science and engineering research. The simplest and most common is the linear system of equations. For example, here is a linear system with two equations and two unknowns:

Slide Type Fragment ▾

$$\begin{aligned}y + 3z &= 16 \\4v - z &= -1\end{aligned}$$

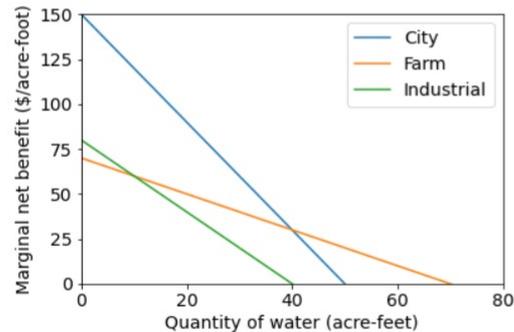
Python for Environmental Research course

In [5]:

```
### plot MNB curves
plt.plot(qs, city_q)
plt.plot(qs, farm_q)
plt.plot(qs, indus_q)
plt.xlim([0, 80])
plt.ylim([0, 150])
plt.xlabel('Quantity of water (acre-feet)')
plt.ylabel('Marginal net benefit (\$/acre-foot)')
plt.legend(['City', 'Farm', 'Industrial'])
```

Slide Type Fragment

Out[5]: <matplotlib.legend.Legend at 0x7f5c7d1487f0>



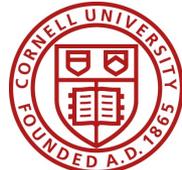
Slide Type Slide

What if there are only 100 acre-feet of water available? What is the efficient allocation to each sector?

Thank you!

INFEWS/T2: The sustainability-productivity tradeoff: Water supply vulnerabilities and adaptation opportunities in California's coupled agricultural and energy sectors, NSF Award #1639268

Greg Characklis, HB Zeff, Pat Reed, Jon Herman, Josué Medellín-Azuara, Jordan Kern, Tamlin Pavelsky, Keyvan Malek, Rohini Gupta



CyberTraining: CIU: Cross-disciplinary Training for Findable, Accessible, Interoperable, and Reusable (FAIR) Science, NSF Award #1829764

Venkatesh Merwade, Matthew Huber, Carol Song, Lan Zhao, Wan Ju Huang, I Luk Kim

