

SOARS 2018 WORKSHOPS

COMPUTATIONAL THINKING AND DATA SCIENCE

Keith E. Maull, PhD

Workshop Motivation



“ The publication of research papers is slowly changing to adapt to the digital age. We envision that in the near future (5–10 years), scientists will use **radically new tools to author papers and disseminate information** about the process and products of their research. These tools will **document** and **publish the computational workflow** as well as all the associated **digital objects** (data, software, etc.) that **form the basis of a paper**.

Gil, Y., et al. (2016), *Toward the Geoscience Paper of the Future: Best practices for documenting and sharing research from data to software to provenance, Earth and Space Science*, 3, 388–415, doi:[10.1002/2015EA000136](https://doi.org/10.1002/2015EA000136).

2018 Computational Thinking and Data Science Workshops

SECTION A(M)

- **Introduction** to computational thinking
- Use **algorithms** solve problems (GCD, search, etc.)
- Develop intermediate solutions with **psuedocode** and converting that psuedocode to **running Python code**
- Apply basic knowledge of tools (Jupyter) and resources

SECTION P(M)

- **Deeper dive** into Python and the data science stack
- Implement **working solutions** to common tasks (data manipulation, graphing, etc.)
- Develop **advanced strategies** and working knowledge of **platforms, tools and workflows** (Jupyter, Python libraries, etc.)

Tools we will use ...

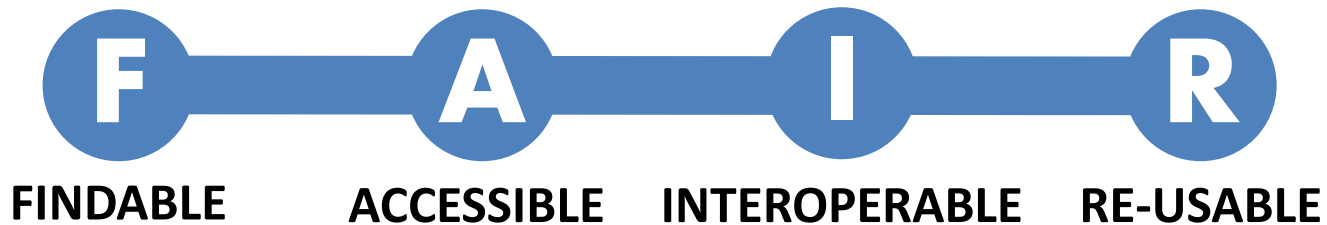
SECTIONS A(M)+P(M)



GitHub



We want our work to be ...



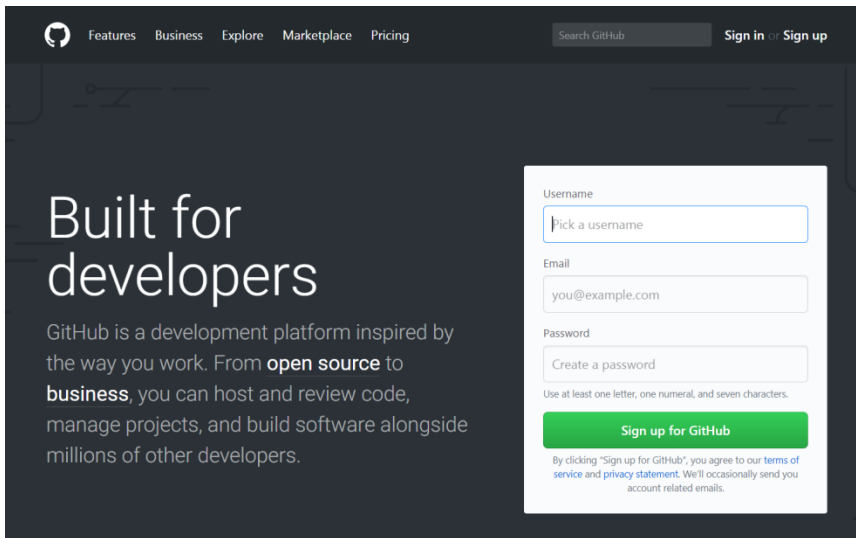
Wilkinson, M. D., Dumontier, M., Aalbersberg, Ij. J., Appleton, G., Axton, M., Baak, A., ... Mons, B. (2016). The FAIR Guiding Principles for scientific data management and stewardship. *Scientific Data*, 3, 160018.

<https://doi.org/bdd4>

3 things you need to do ...

1

GET A FREE GITHUB ACCOUNT

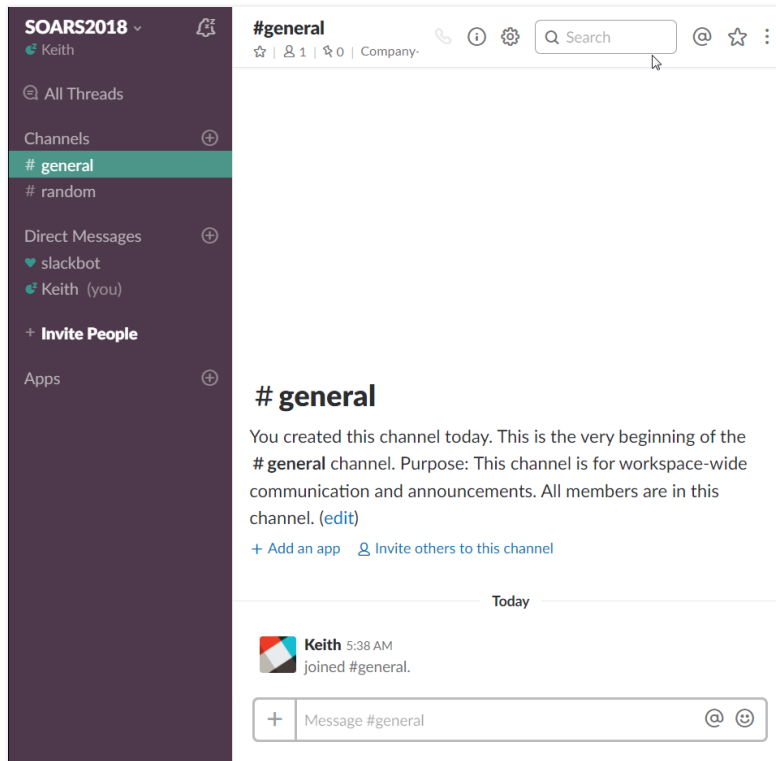
A screenshot of the GitHub website's sign-up page. The page has a dark background with the GitHub logo and navigation links (Features, Business, Explore, Marketplace, Pricing) at the top. The main heading is "Built for developers". Below it, a paragraph describes GitHub as a development platform inspired by the way you work, from open source to business. On the right side, there is a white sign-up form with fields for Username (placeholder: "Pick a username"), Email (placeholder: "you@example.com"), and Password (placeholder: "Create a password"). Below the password field, there is a note: "Use at least one letter, one numeral, and seven characters." A green button labeled "Sign up for GitHub" is at the bottom of the form. Below the button, there is a small disclaimer: "By clicking 'Sign up for GitHub', you agree to our terms of service and privacy statement. We'll occasionally send you account related emails."

- Go to Set up a Github account at <https://github.com> (make sure to use your .edu email address!)
- Send me (kmaull@ucar.edu) your Github ID
- Bookmark the repository for this year's workshop (<https://git.io/vAa7p>)
- Install GithubDesktop (<https://desktop.github.com>) for Win/Mac
- Browse around Github and watch a tutorial!

3 things you need to do ...

2

JOIN OUR SLACK CHANNEL



- Go to <https://soarshq18.slack.com> and set up a free account on our channel
- Send me (kmaull@ucar.edu) if you have trouble getting on to the channel
- Watch a video / tutorial about slack (there is one when you login)

3 things you need to do ...

3

FAMILIARIZE/RE- ACQUAINT YOURSELF WITH PYTHON



- Skim a few of the online resources in the syllabus (on Github)
- <https://python.org!>
- You do **not** need to install Python on your computer, but if you do, install Anaconda from <https://anaconda.com>

Things to watch for ...

1

INFORMATION ABOUT OUR JUPYTER ENVIRONMENT



- I should be sending an email out soon
- You can look at **prior workshops** to see what Jupyter is all about
- You will **not** need to install anything, **but** if you **want to play on your own machine**, do **contact me**

Things you might also do ...

- Read the paper:
 - *Gil, Y., et al. (2016), Toward the Geoscience Paper of the Future: Best practices for documenting and sharing research from data to software to provenance, Earth and Space Science, 3, 388–415, doi:[10.1002/2015EA000136](https://doi.org/10.1002/2015EA000136).*
- Explore the awesome Github repository `Python for the Geosciences`:
 - <https://git.io/vhLhr>
- Check out Jupyter Notebooks examples
 - <http://nb.bianp.net/sort/views/>
- Check out some of the prior workshops:
 - <https://git.io/v6XyK> (2016)
 - <https://git.io/vHqof> (2017)

Some inspiration ...

Here is a paper ...
actually a **pre-print**

The screenshot displays the journal's website for 'Atmospheric Chemistry and Physics'. The header includes the journal title, a subtitle 'An interactive open-access journal of the European Geosciences Union', and the EGU logo. Navigation links for 'EGU.eu', 'EGU Journals', 'EGU Highlight Articles', 'Contact', and 'Imprint' are provided. A sidebar on the left contains links for 'Submit a manuscript', 'Manuscript tracking', 'About', 'Editorial & advisory board', 'Articles', 'Special issues', 'Highlight articles', 'Subscribe to alerts', 'Peer review', 'For authors', and 'For reviewers'. The main content area features a 'Discussion papers' section with tabs for 'Abstract', 'Assets', 'Discussion', and 'Metrics'. The article title is 'Effective radiative forcing in the aerosol-climate model CAM5.3-MARC-ARG'. The authors listed are Benjamin S. Grandey¹, Daniel Rothenberg², Alexander Avramov^{2,3}, Qinjiao Jin², Hsiang-He Lee¹, Xiaohong Liu⁴, Zheng Lu⁴, Samuel Albeni^{5,6}, and Chien Wang^{2,1}. The page indicates it is a preprint under review for the journal. The 'Journal metrics' section shows various scores: IF 5.318, IF 5-year 5.896, CiteScore 5.72, SNIP 1.330, SJR 3.207, IPP 4.756, and h5-index 89. The 'Download' section offers PDF and XML files, with a supplement of 6128 KB. A 'Short summary' and 'Citation' section are also present, along with social media sharing options.

Atmospheric Chemistry and Physics
An interactive open-access journal of the European Geosciences Union

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<https://doi.org/10.5194/acp-2018-118>
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Research article

02 May 2018

Review status

This discussion paper is a preprint. It is a manuscript under review for the Journal Atmospheric Chemistry and Physics (ACP).

Effective radiative forcing in the aerosol-climate model CAM5.3-MARC-ARG

Benjamin S. Grandey¹, Daniel Rothenberg², Alexander Avramov^{2,3}, Qinjiao Jin², Hsiang-He Lee¹, Xiaohong Liu⁴, Zheng Lu⁴, Samuel Albeni^{5,6}, and Chien Wang^{2,1}

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³Department of Environmental Sciences, Emory University, Atlanta, Georgia, USA
⁴Department of Atmospheric Science, University of Wyoming, Laramie, Wyoming, USA
⁵Department of Earth and Atmospheric Sciences, Cornell University, Ithaca, New York, USA
⁶Laboratoire des Sciences du Climat et de l'Environnement, LSCE/IPSL, CEA-CNRS-UVSQ, Gif-sur-Yvette, France

Received: 01 Feb 2018 – Accepted for review: 01 May 2018 – Discussion started: 02 May 2018

Abstract. We quantify the effective radiative forcing (ERF) of anthropogenic aerosols modelled by the aerosol-climate model CAM5.3-MARC-ARG. CAM5.3-MARC-ARG is a new configuration of the Community Atmosphere Model version 5.3 (CAM5.3) in which the default aerosol module has been replaced by the two-Moment, Multi-Modal, Mixing-state-resolving Aerosol model for Research of Climate (MARC). CAM5.3-MARC-ARG uses the default ARG aerosol

Search articles

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Short summary

Citation

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Some inspiration ...

This paper includes
analysis ... done with
some **data** and **code**



Effective radiative forcing in the aerosol-climate model CAM5.3-MARC-ARG

Benjamin S. Grandey et al.

Supplement

<https://doi.org/10.5194/acp-2018-118-supplement>

Data sets

Data for "Effective radiative forcing in the aerosol-climate model CAM5.3-MARC-ARG"

B. S. Grandey

<https://doi.org/10.6084/m9.figshare.5687812>

Model code and software

Configuration and analysis for "Effective radiative forcing in the aerosol-climate model CAM5.3-MARC-ARG"

B. S. Grandey

<https://doi.org/10.5281/zenodo.1239247>

MARC - Model for Research of Aerosols and Climate

A. Avramov, D. Rothenberg, Q. Jin, S. Garimella, B. Grandey, and C. Wang

<https://doi.org/10.5281/zenodo.1117370>

Some inspiration ...

The data is findable here:

<https://doi.org/10.6084/m9.figshare.5687812>

The screenshot shows a Figshare dataset page. At the top, there is a list of files: `so4_elev_p17c_marc_2000.nc`, `so4_surf_p17c_marc_1850.nc`, and `so4_surf_p17c_marc_2000.nc`. Below the file list, there are buttons for **Cite**, **Download all (16.41 GB)**, **Share**, **Embed**, and **+ Collect (you need to log in first)**. The page title is **Data for "Effective radiative forcing in the aerosol-climate model CAM5.3-MARC-ARG"**. It indicates **Version 2** was published on 31.01.2018, 20:08 by Benjamin S. Grandey. The page shows 203 views, 38 downloads, and 1 citation. An introduction section states that the data accompany a manuscript titled "Effective radiative forcing in the aerosol-climate model CAM5.3-MARC-ARG" by B. S. Grandey, D. Rothenberg, A. Avramov, Q. Jin, H.-H. Lee, X. Liu, Z. Lu, S. Albani, and C. Wang. The files contain input data and output data associated with the CESM-CAM5 climate model simulations described in the manuscript. A link is provided to <https://github.com/grandey/p17c-marc-comparison/> for details of the experimental design, model configuration, data management, and analysis. On the right, there is a circular badge with the number 1, a list of categories including Atmospheric Sciences, Atmospheric Aerosols, Atmospheric Radiation, Climate Science, and Climate Change Processes, and a list of keywords including aerosol and radiative forcing.

so4_elev_p17c_marc_2000.nc
so4_surf_p17c_marc_1850.nc
so4_surf_p17c_marc_2000.nc

↓

Cite **Download all (16.41 GB)** **Share** **Embed** **+ Collect (you need to log in first)** 1 / 191 < > ☐ ☰

Data for "Effective radiative forcing in the aerosol-climate model CAM5.3-MARC-ARG"

Version 2 31.01.2018, 20:08 by Benjamin S. Grandey

203 views | **38** downloads | **1** citations

Introduction:

These data accompany the manuscript titled "Effective radiative forcing in the aerosol-climate model CAM5.3-MARC-ARG" by B. S. Grandey, D. Rothenberg, A. Avramov, Q. Jin, H.-H. Lee, X. Liu, Z. Lu, S. Albani, and C. Wang. The files contain input data and output data associated with the CESM-CAM5 climate model simulations described in the manuscript.

Please also see <https://github.com/grandey/p17c-marc-comparison/> for details of the experimental design, model configuration, data management, and

CATEGORIES

- Atmospheric Sciences
- Atmospheric Aerosols
- Atmospheric Radiation
- Climate Science
- Climate Change Processes

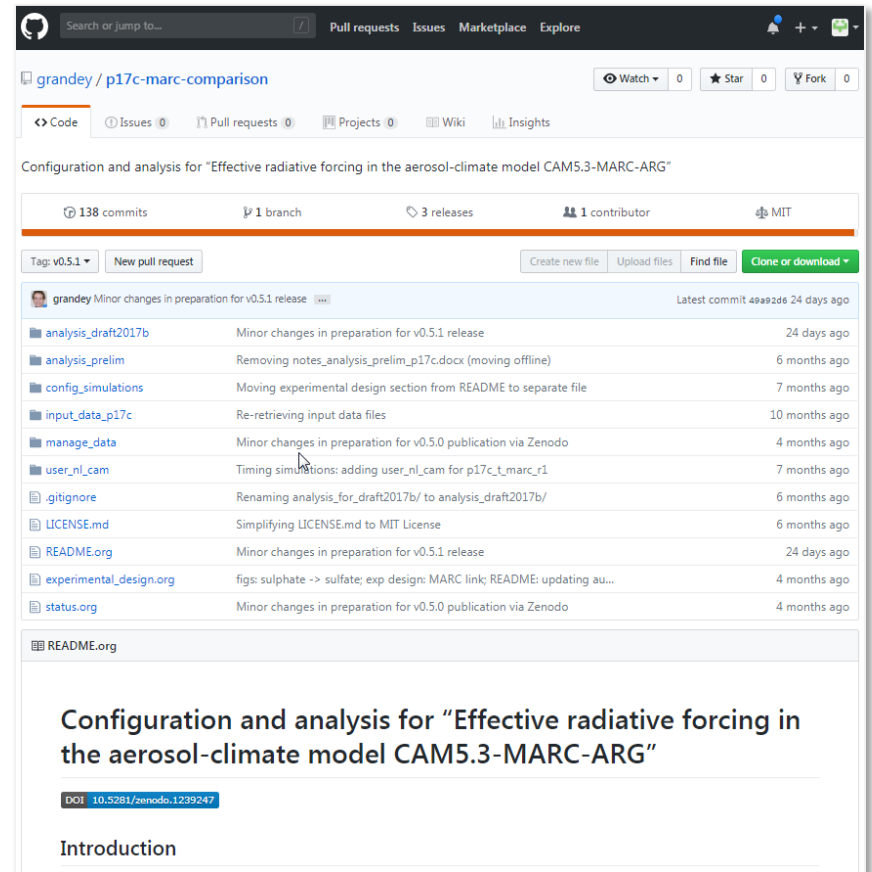
KEYWORD(S)

aerosol radiative forcing

Some inspiration ...

The code is also
findable here:

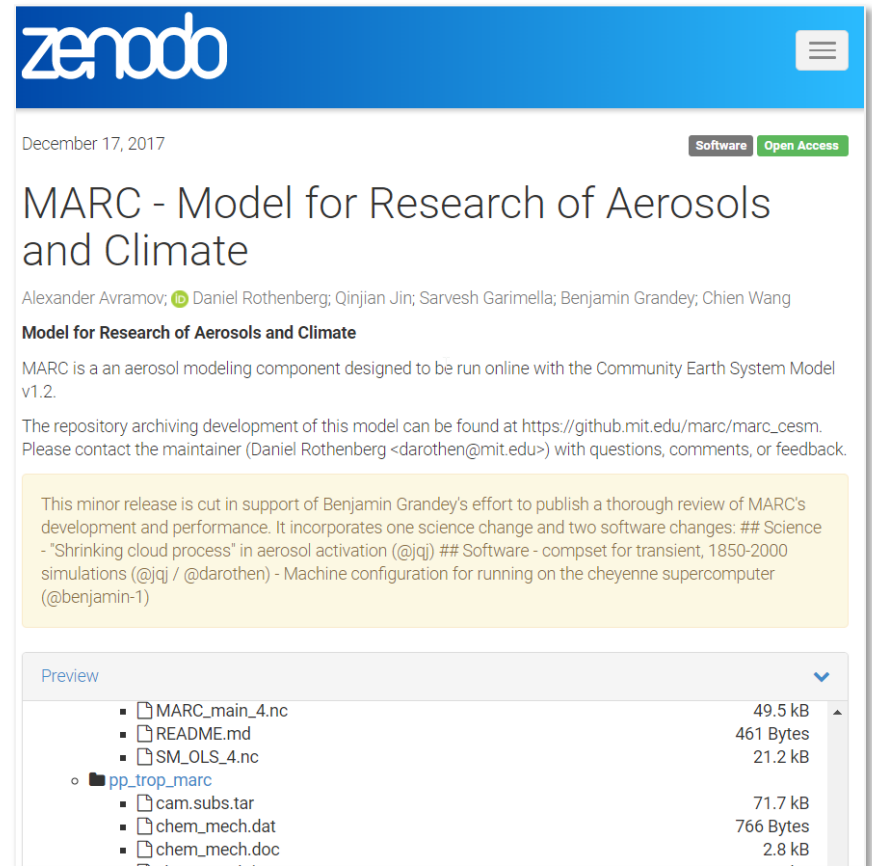
<https://doi.org/10.5281/zenodo.1239247>



Some inspiration ...

The model code upon
which this work is
build is here ...

<https://doi.org/10.5281/zenodo.1117370>



The screenshot shows the Zenodo repository page for the MARC model. The page has a blue header with the Zenodo logo. Below the header, the date "December 17, 2017" is displayed on the left, and "Software" and "Open Access" badges are on the right. The title "MARC - Model for Research of Aerosols and Climate" is prominently displayed. The authors listed are Alexander Avramov, Daniel Rothenberg, Qinqian Jin, Sarvesh Garimella, Benjamin Grandey, and Chien Wang. The subtitle is "Model for Research of Aerosols and Climate". The description states that MARC is an aerosol modeling component designed to be run online with the Community Earth System Model v1.2. It also provides a link to the GitHub repository and contact information for the maintainer. A yellow box contains a note about a minor release. At the bottom, a "Preview" section shows a file tree with items like MARC_main_4.nc, README.md, SM_OLS_4.nc, and a subdirectory pp_trop_marc containing cam.subs.tar, chem_mech.dat, and chem_mech.doc, along with their respective sizes.

zenodo

December 17, 2017 Software Open Access

MARC - Model for Research of Aerosols and Climate

Alexander Avramov, Daniel Rothenberg, Qinqian Jin, Sarvesh Garimella, Benjamin Grandey, Chien Wang

Model for Research of Aerosols and Climate

MARC is an aerosol modeling component designed to be run online with the Community Earth System Model v1.2.

The repository archiving development of this model can be found at https://github.mit.edu/marc/marc_cesm. Please contact the maintainer (Daniel Rothenberg <darochen@mit.edu>) with questions, comments, or feedback.

This minor release is cut in support of Benjamin Grandey's effort to publish a thorough review of MARC's development and performance. It incorporates one science change and two software changes: ## Science - "Shrinking cloud process" in aerosol activation (@jqj) ## Software - compset for transient, 1850-2000 simulations (@jqj / @darochen) - Machine configuration for running on the cheyenne supercomputer (@benjamin-1)

Preview

- MARC_main_4.nc 49.5 kB
- README.md 461 Bytes
- SM_OLS_4.nc 21.2 kB
- pp_trop_marc
 - cam.subs.tar 71.7 kB
 - chem_mech.dat 766 Bytes
 - chem_mech.doc 2.8 kB

Some inspiration ...

And if that wasn't enough ...

Acknowledgements

This research is supported by the National Research Foundation of Singapore under its Campus for Research Excellence and Technological Enterprise programme. The Center for Environmental Sensing and Modeling is an interdisciplinary research group of the Singapore-MIT Alliance for Research and Technology. This research is also supported by the U.S. National Science Foundation (AGS-1339264) and the U.S. Department of Energy, Office of Science (DE-FG02-94ER61937). The CESM project is supported by the National Science Foundation and the Office of Science (BER) of the U.S. Department of Energy. We acknowledge high-performance computing support from Cheyenne ([doi:10.5065/D6RX99HX](https://doi.org/10.5065/D6RX99HX)) provided by NCAR's Computational and Information Systems Laboratory, sponsored by the National Science Foundation. We thank Natalie Mahowald for contributing dust model code, optical tables, a soil erodibility map, and advice, all of which have aided the development of CAM5.3-MARC-ARG.

Wow!

A person wearing a red and yellow jumpsuit is captured mid-leap from a rocky, snow-covered cliff. They are falling into a deep blue body of water. In the background, a range of jagged, snow-capped mountains rises under a clear sky. The scene is set during the day, with sunlight illuminating the snow and the person's gear.

You got this!