

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 ...

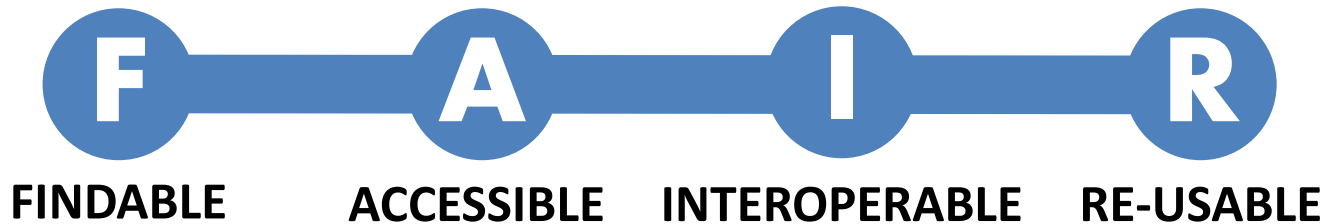
SECTIONS A(M)+P(M)



GitHub



We want our work to be ...



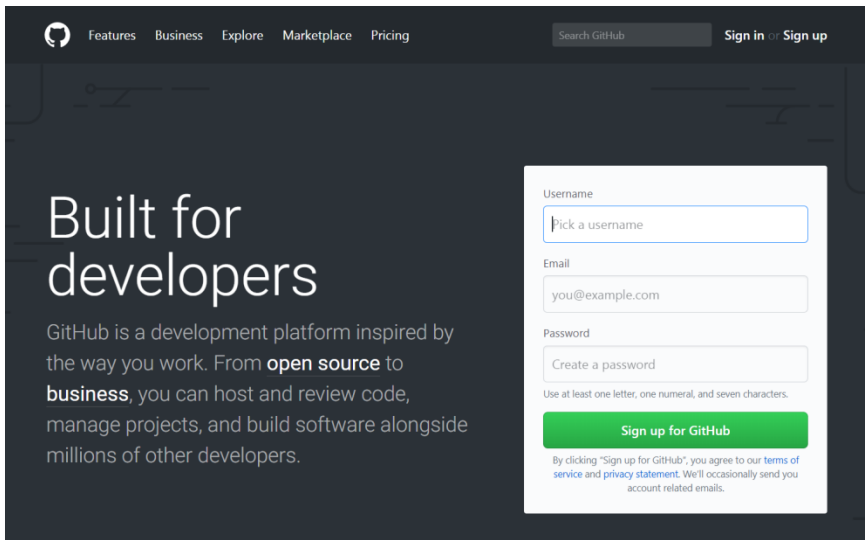
Wilkinson, M. D., Dumontier, M., Aalbersberg, Ij. J., Appleton, G., Axton, M., Baak, A., ... Mons, B. (2016). The FAIR Guiding Principles for scientific data management and stewardship. *Scientific Data*, 3, 160018.

<https://doi.org/bdd4>

3 things you need to do ...

1

GET A FREE GITHUB ACCOUNT

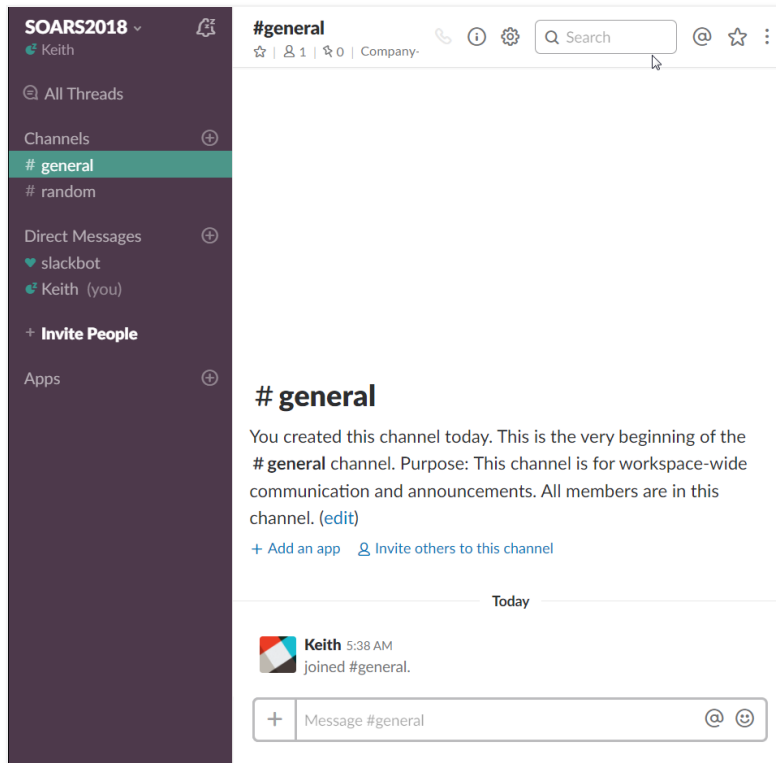
A screenshot of the GitHub website's sign-up page. The page has a dark background with white text. At the top, there are navigation links: Features, Business, Explore, Marketplace, Pricing, and a search bar. Below the navigation, the text reads "Built for developers" and "GitHub is a development platform inspired by the way you work. From open source to business, you can host and review code, manage projects, and build software alongside millions of other developers." On the right side, there is a white sign-up form with fields for Username, Email, and Password. The Username field contains the placeholder text "Pick a username". The Email field contains "you@example.com". The Password field contains the placeholder text "Create a password". Below the password field, there is a note: "Use at least one letter, one numeral, and seven characters." At the bottom of the form is a green button labeled "Sign up for GitHub". 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 shows the article page for "Effective radiative forcing in the aerosol-climate model CAM5.3-MARC-ARG" in the journal Atmospheric Chemistry and Physics. The page is marked as a pre-print under review. It includes a navigation menu, a sidebar with journal metrics, and a main content area with the title, authors, abstract, and download options. The journal metrics sidebar lists various indices such as Clarivate Analytics IF 5.318, Scopus CiteScore 5.72, and h5-index 89. The main content area includes the title, authors (Benjamin S. Grandey et al.), a short summary, and a share section with social media icons.

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

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Discussion papers

Abstract | Assets | Discussion | Metrics

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}, Qinjian Jin⁴, Hsiang-He Lee¹, Xiaohong Liu⁴, Zheng Lu⁴, Samuel Alban^{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
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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

User ID: Password: New user? | Lost login?

Journal metrics

Clarivate Analytics	IF 5.318
Clarivate Analytics	IF 5-year 5.896
Scopus	CiteScore 5.72
CWTS	SNIP 1.330
SJR	SJR 3.207
CWTS	IPP 4.756
h5-index	89

Search articles

Download

Supplement (6128 KB)

Short summary

Anthropogenic emissions of aerosol particles likely cool the climate system. We investigate... Read more

Citation

BibTeX | EndNote

Share

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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 data 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 shows 203 views, 38 downloads, and 1 citation. The version is 'Version 2' from 31.01.2018, 20:08 by Benjamin S. Grandey. The introduction text reads: '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'. The categories listed are Atmospheric Sciences, Atmospheric Aerosols, Atmospheric Radiation, Climate Science, and Climate Change Processes. The keywords are aerosol and radiative forcing.

Some inspiration ...

The code is also
findable here:

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

A screenshot of a GitHub repository page for 'grandey / p17c-marc-comparison'. The repository is titled 'Configuration and analysis for "Effective radiative forcing in the aerosol-climate model CAM5.3-MARC-ARG"'. It shows 138 commits, 1 branch, 3 releases, and 1 contributor. The repository is licensed under MIT. A list of files is displayed, including 'analysis_draft2017b', 'analysis_prelim', 'config_simulations', 'input_data_p17c', 'manage_data', 'user_nl_cam', '.gitignore', 'LICENSE.md', 'README.org', 'experimental_design.org', and 'status.org'. The README section is visible at the bottom, showing the title and DOI: 10.5281/zenodo.1239247.

grandey / p17c-marc-comparison

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

138 commits 1 branch 3 releases 1 contributor MIT

Tag: v0.5.1 New pull request Create new file Upload files Find file Clone or download

File	Description	Last commit
analysis_draft2017b	Minor changes in preparation for v0.5.1 release	24 days ago
analysis_prelim	Removing notes_analysis_prelim_p17c.docx (moving offline)	6 months ago
config_simulations	Moving experimental design section from README to separate file	7 months ago
input_data_p17c	Re-retrieving input data files	10 months ago
manage_data	Minor changes in preparation for v0.5.0 publication via Zenodo	4 months ago
user_nl_cam	Timing simulations: adding user_nl_cam for p17c_t_marc_r1	7 months ago
.gitignore	Renaming analysis_for_draft2017b/ to analysis_draft2017b/	6 months ago
LICENSE.md	Simplifying LICENSE.md to MIT License	6 months ago
README.org	Minor changes in preparation for v0.5.1 release	24 days ago
experimental_design.org	figs: sulphate -> sulfate; exp design: MARC link; README: updating au...	4 months ago
status.org	Minor changes in preparation for v0.5.0 publication via Zenodo	4 months ago

README.org

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

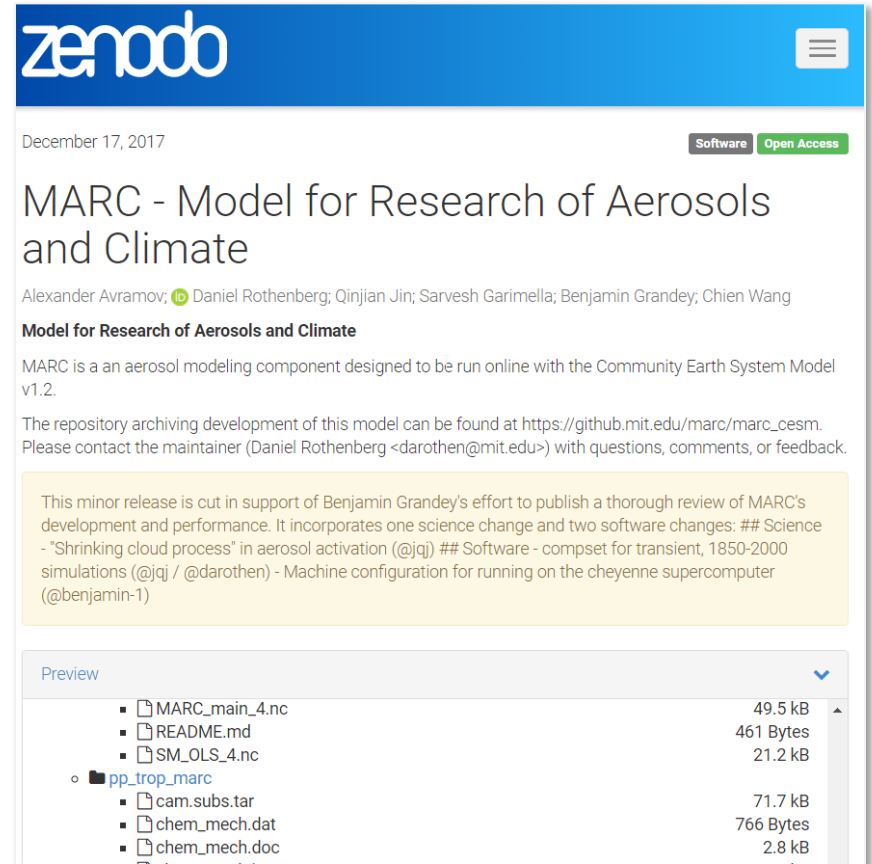
DOI: 10.5281/zenodo.1239247

Introduction

Some inspiration ...

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

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



The screenshot shows a Zenodo repository page for the MARC model. The page header includes the Zenodo logo and a navigation menu. The main content area displays the title "MARC - Model for Research of Aerosols and Climate" and the authors: Alexander Avramov, Daniel Rothenberg, Qinjian Jin, Sarvesh Garimella, Benjamin Grandey, and Chien Wang. Below the title, there is a description of the model and a link to the GitHub repository. A yellow callout box highlights a minor release update. At the bottom, a "Preview" section shows a file tree with the following items:

File Name	Size
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

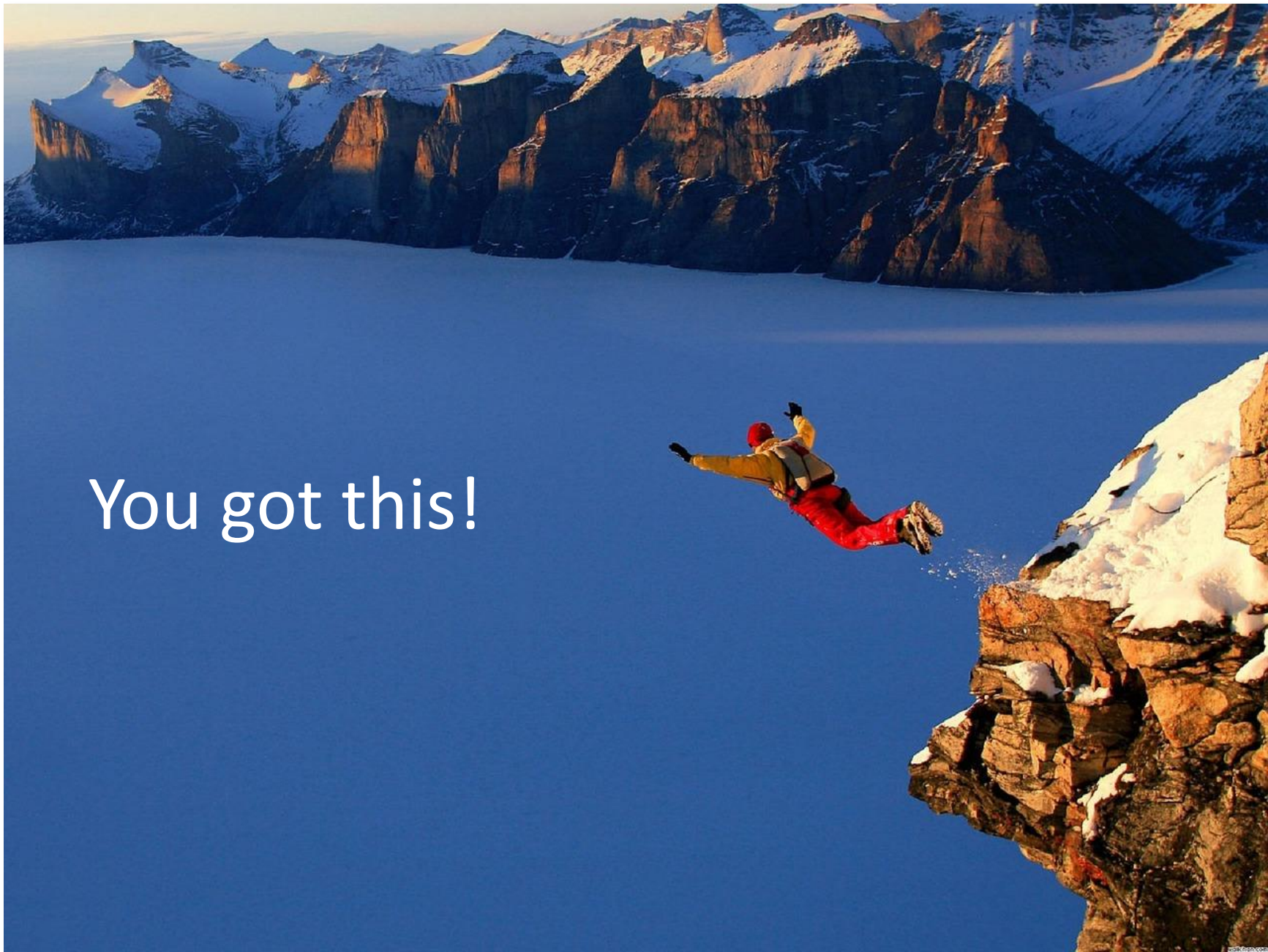
Some inspiration ...

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!



You got this!