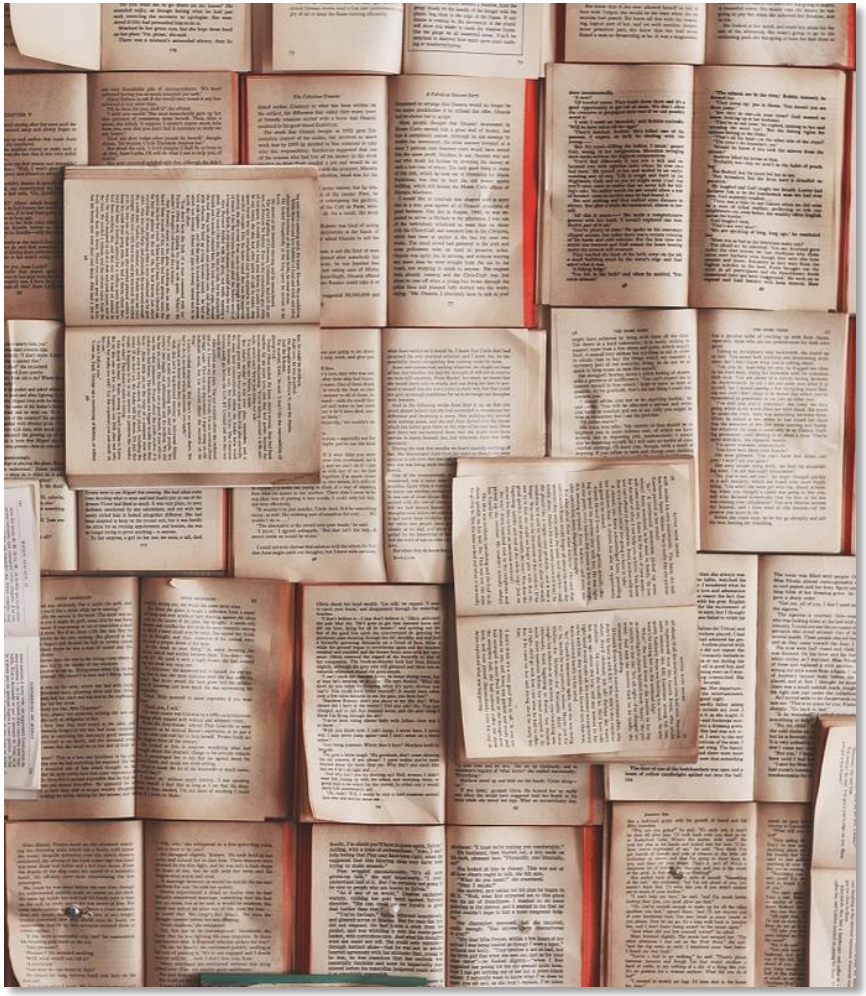
# SOARS 2018 WORKSHOPS

## COMPUTATIONAL THINKING AND DATA SCIENCE

Keith E. Maull, PhD

# Workshop Motivation



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> 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.*

# 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.)

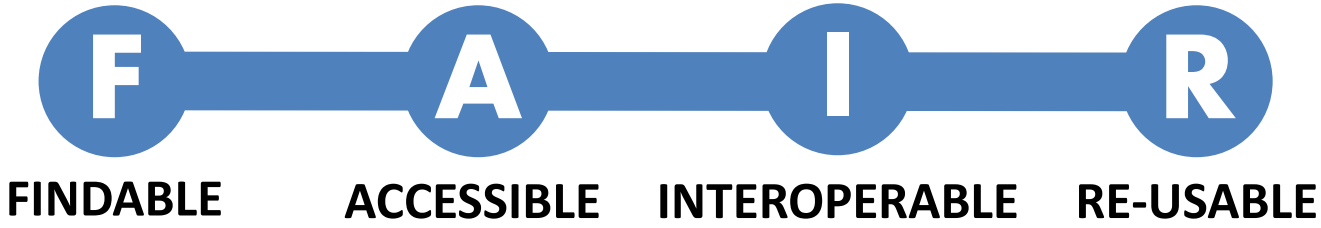
# Tools we will use …

SECTIONS A(M)+P(M)





# We want our work to be …

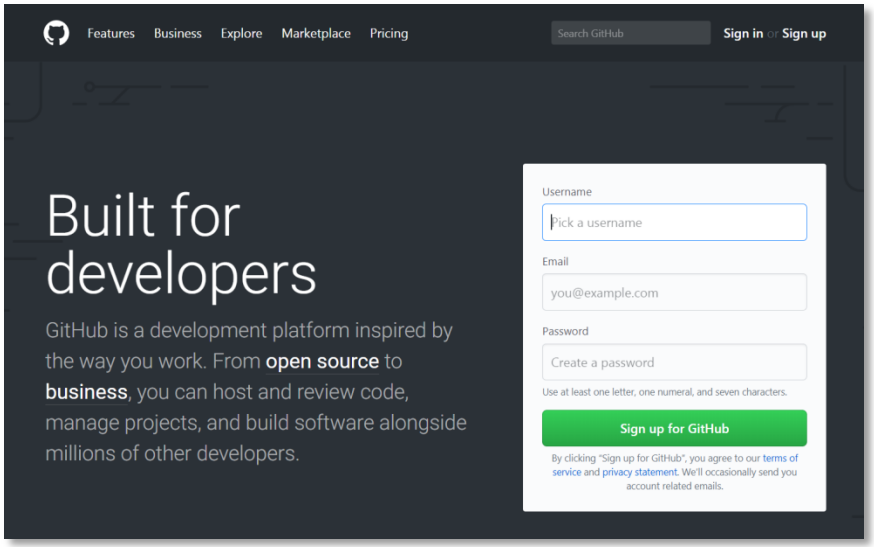



Wilkinson, M. D., Dumontier, M., Aalbersberg, Ij. J., Appleton, G., Axton, M., Baak, A., … Mons, B. (2016). The FAIR Guiding Principles for scientific data management and stewardship. Scientific Data, 3, 160018. https://doi.org/bdd4

# 3 things you need to do …

1

## GET A FREE GITHUB ACCOUNT

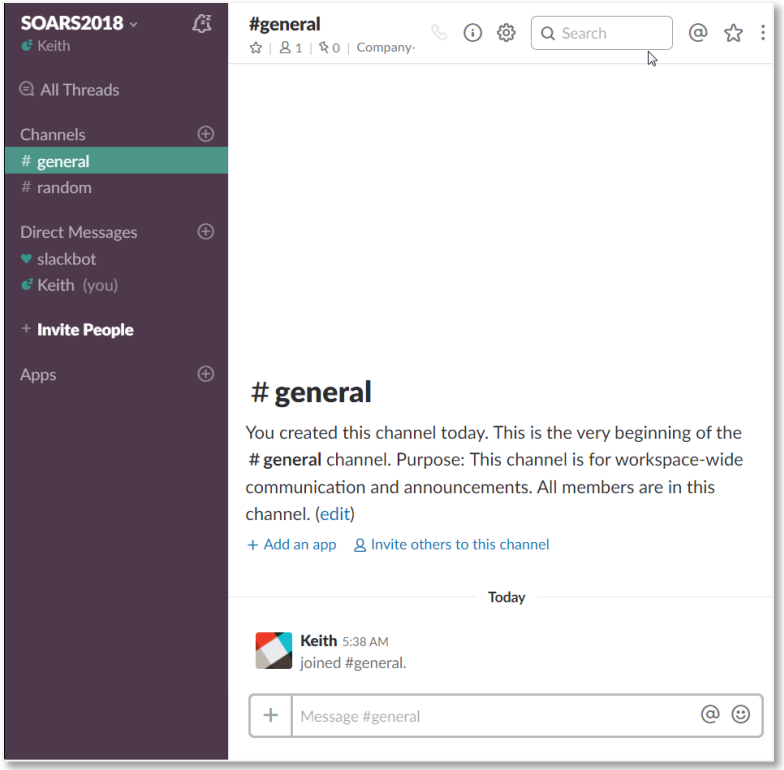



- Go to Set up a Github account at https://github.com **(make sure to use your .edu email address!)**
- **Send me (kmaull@ucar.edu) your Github ID**
- Bookmark the repository for this year's workshop (https://git.io/vAa7p)
- Install GithubDesktop (https://desktop.github.com) for Win/Mac
- Browse around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

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

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h5-index 89

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. Grandey[1], Daniel Rothenberg[2], Alexander Avramov[2,3], Qinjian Jin[2], Hsiang-He Lee[1], Xiaohong Liu[4], Zheng Lu[4], Samuel Albani[5,6], and Chien Wang[2,1]
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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

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Anthropogenic emissions of aerosol particles likely cool the climate system. We investigate…
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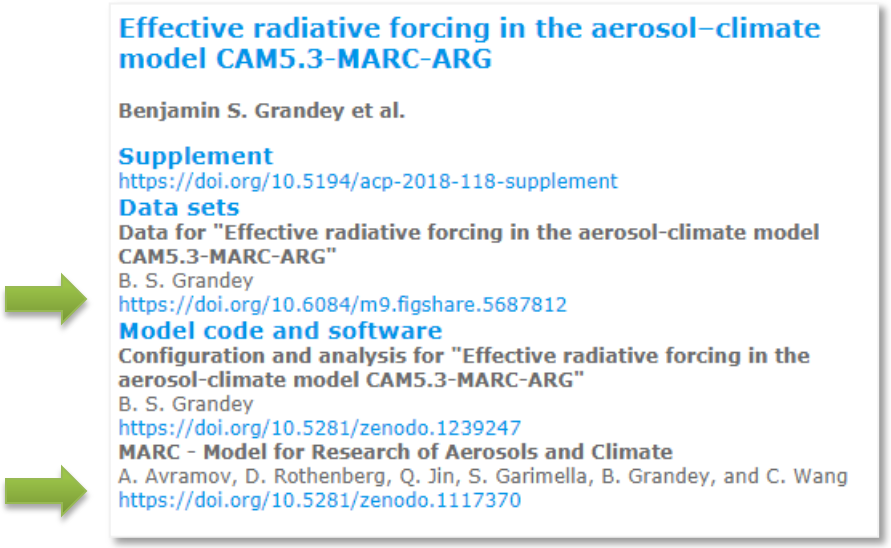
# Some inspiration …

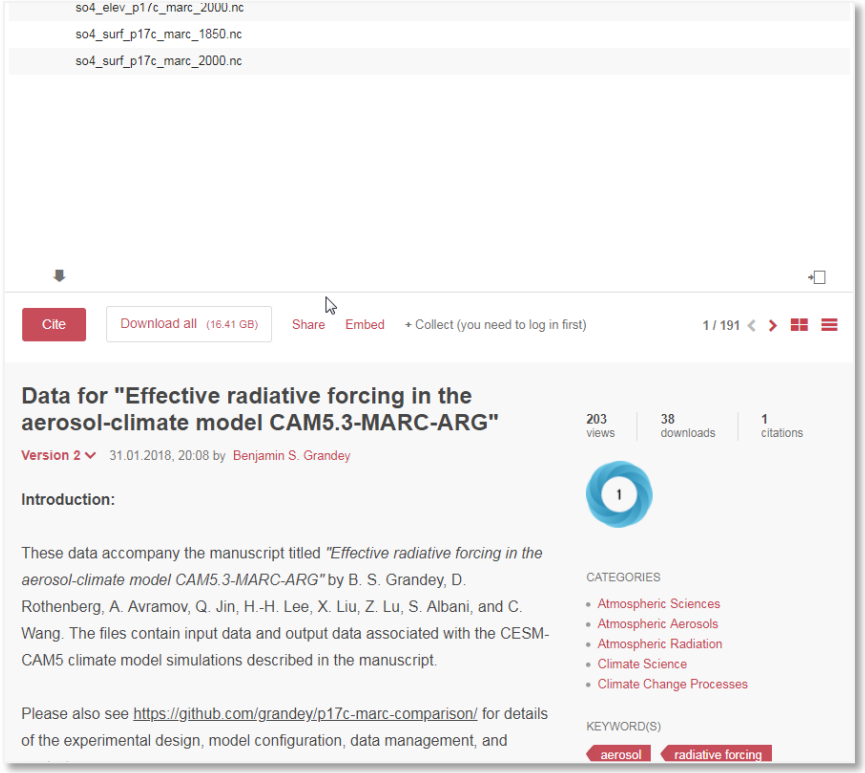
This paper includes **analysis** … done with some **data** and **code**



# Some inspiration …

The **data is findable** here:

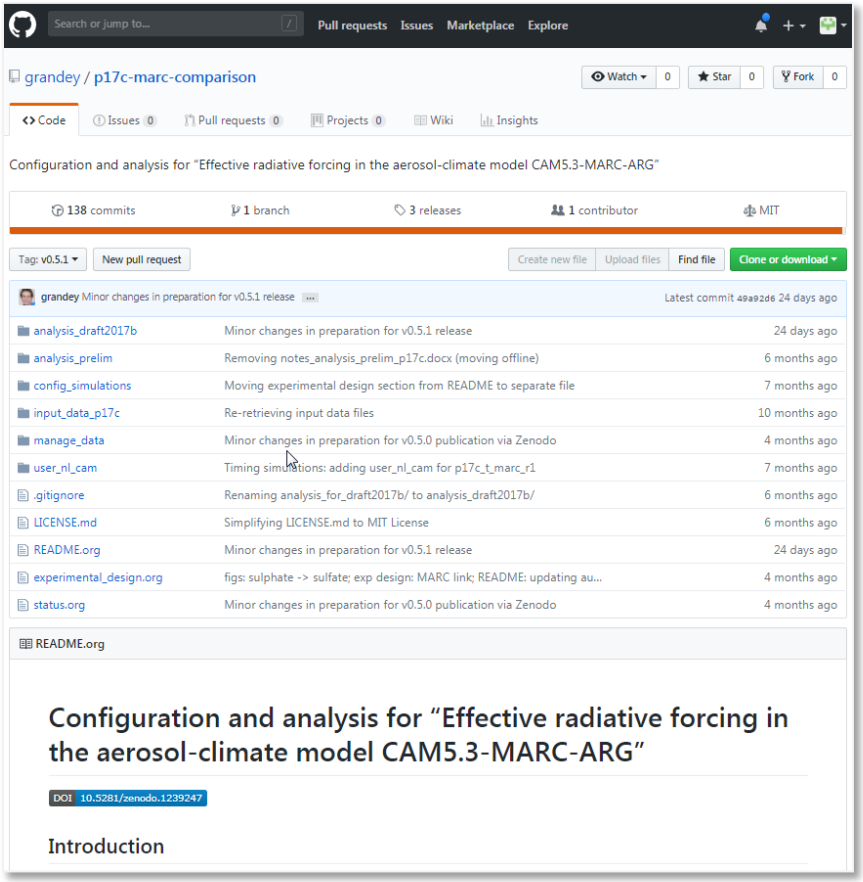
https://doi.org/10.6084/m9.figshare.5687812



# Some inspiration …

The **code is also findable** here:

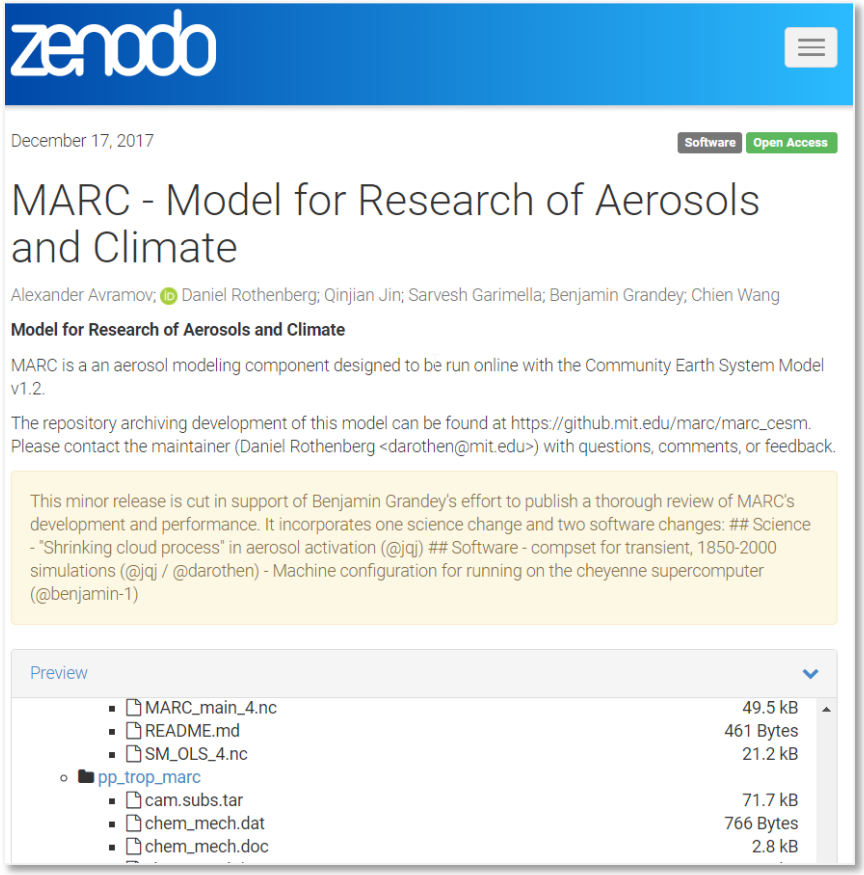
https://doi.org/10.5281/zenodo.1239247



# Some inspiration …

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

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



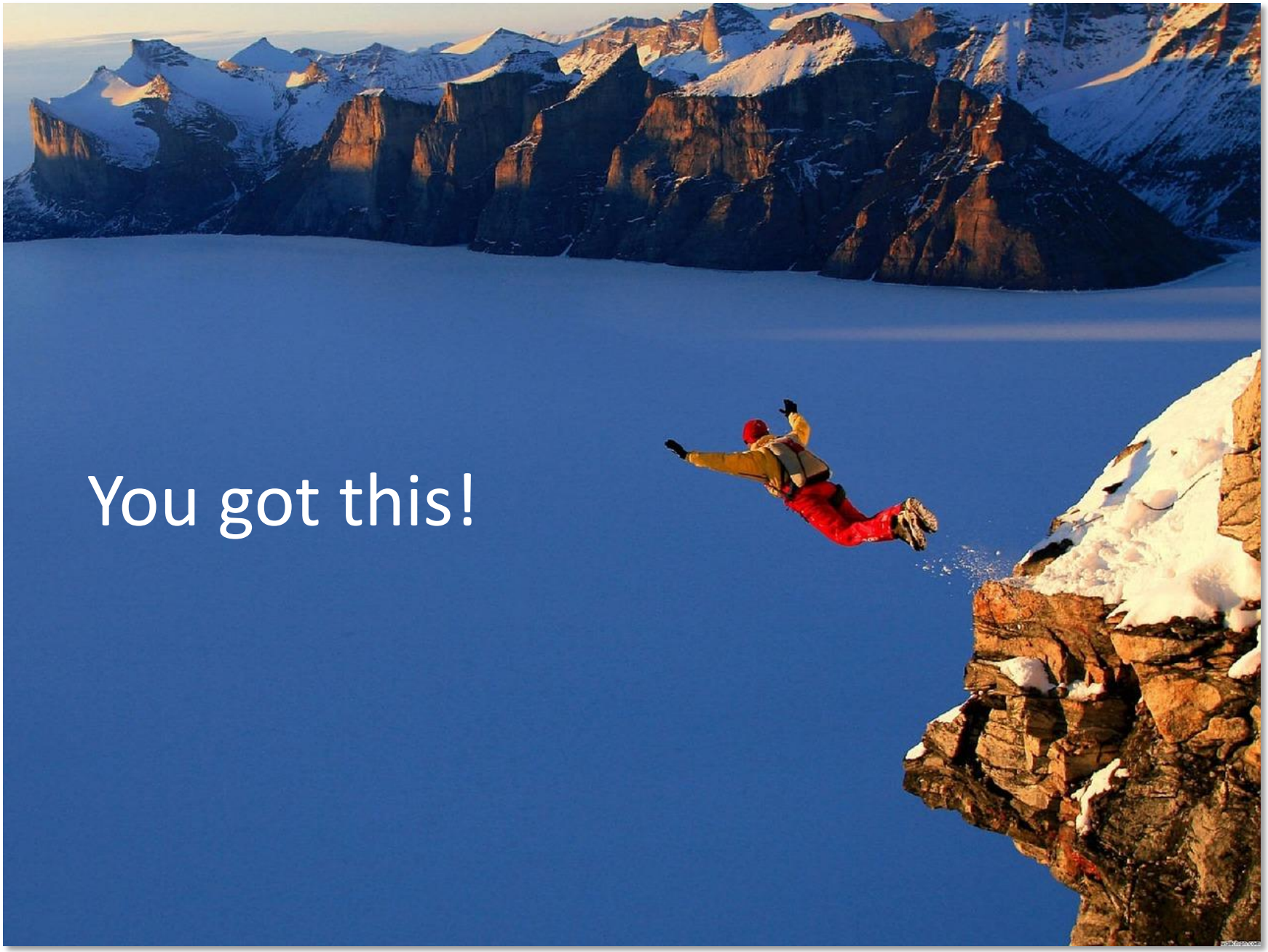
# Some inspiration …

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) 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!**

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