

Introductory Remarks

Best Practices Workshop, March 25-26 2019, Hampton VA

Carlos Cruz
Jules Kouatchou
Brent Smith

NASA GSFC Code 606/610 (ASTG/GMAO)
Greenbelt, Maryland 20771

Who are we?

- Carlos Cruz (Computational Scientist - ASTG)
- Jules Kouatchou (Computational Scientist - ASTG)
- Brent Smith (Computational Scientist- GMAO)



Objectives of this tutorial

To provide an overview of **useful** software engineering practices to HPC code developers



Best Practices for Scientific Computing

OPEN ACCESS Freely available online



Community Page

Best Practices for Scientific Computing

Greg Wilson^{1*}, D. A. Aruliah², C. Titus Brown³, Neil P. Chue Hong⁴, Matt Davis⁵, Richard T. Guy^{6a}, Steven H. D. Haddock⁷, Kathryn D. Huff⁸, Ian M. Mitchell⁹, Mark D. Plumbley¹⁰, Ben Waugh¹¹, Ethan P. White¹², Paul Wilson¹³

1 Mozilla Foundation, Toronto, Ontario, Canada, **2** University of Ontario Institute of Technology, Oshawa, Ontario, Canada, **3** Michigan State University, East Lansing, Michigan, United States of America, **4** Software Sustainability Institute, Edinburgh, United Kingdom, **5** Space Telescope Science Institute, Baltimore, Maryland, United States of America, **6** University of Toronto, Toronto, Ontario, Canada, **7** Monterey Bay Aquarium Research Institute, Moss Landing, California, United States of America, **8** University of California Berkeley, Berkeley, California, United States of America, **9** University of British Columbia, Vancouver, British Columbia, Canada, **10** Queen Mary University of London, London, United Kingdom, **11** University College London, London, United Kingdom, **12** Utah State University, Logan, Utah, United States of America, **13** University of Wisconsin, Madison, Wisconsin, United States of America



Best Practices for Scientific Computing

1. Write programs for people, not computers **Coding standards**
2. Let the computers do the work **make, cmake**
3. Make incremental changes **Git, testing**
4. Don't repeat yourself (or others) **Coding standards**
5. Plan for mistakes **Testing**
6. Optimize software only after it works correctly **Use profilers**
7. Document design and purpose, not mechanics **Documentation**
8. Collaborate **Agile methodology, GitHub**



Agenda

Day 1

- **Introductory Remarks**
- Version Control
- Documentation
- Coding Standards

Day 2

- Agile Development
- Unit Testing and TDD
- Continuous Integration
- Regression Testing
- Containers

