

Software Engineering Updates

Land Ice Working Group

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Outline

- Derecho Overview
- Running CISM and CESM on Derecho
- Diagnostics Efforts
- Other Updates



DALL-E 2 prompt: A glacier scientist at work



Derecho Overview

- Cray supercomputer with 19.87 petaflop performance that is expected to deliver about 3.5x the throughput of the retired Cheyenne machine.
- Includes 2488 compute nodes with 128 AMD cores per node and 82 nodes with 4 NVIDIA GPUs.
- PBS queuing, access to campaign and glade file systems, Intel, Cray and Gnu compilers available, and built-in python and conda environments.



Prompt: A glacier scientist working with the Derecho supercomputer



Derecho Overview

- CISL documentation: <u>https://arc.ucar.edu/knowledge_base/743178</u> <u>33</u>
- "Derecho users can expect to see a 1.3x improvement over the Cheyenne system's performance on a core-for-core basis. Therefore, to estimate how many CPU corehours will be needed for a project on Derecho, multiply the total for a Cheyenne project by 0.77."
- Project numbers and allocations available on Derecho:
 - P93300601: 7.9 million CH currently
 - P93300301: 11.3 million CH currently



Prompt: A glacier scientist at work, sigma 85mm F/1.4



Running CISM on Derecho

- Information on using Derecho is available on the Land Ice Working Group shared Google Drive under "Derecho" or using this link:
 - <u>https://drive.google.com/drive/folders/1p</u>
 <u>eJTokZgUSXD3FPzID5G3EJPiZnYxy1</u>
 <u>q?usp=drive_link</u>
- CISM stand-alone supports Derecho build and testing as of November 28, 2023 or tag cism_main_2.01.013 <u>https://github.com/ESCOMP/CISM/releases/</u> tag/cism_main_2.01.013



Prompt: A digital painting of a glacier scientist working



Running CISM on Derecho

- Building and running is basically the same as on Cheyenne, except Intel is now the preferred default compiler (tag includes improved Intel build speeds).
- Nodes now have 128 cores (increase from 32), queues have different names and there is no "economy" or "share" queue any more.
- New workspaces: /glade/derecho/scratch /glade/campaign/cesm/development/liwg /glade/campaign/cesm/community/liwg
- Data from /glade/p moved to /glade/campaign



Prompt: A vibrant photo of a glacier scientist at sunset, wide angle lens



Running CESM on Derecho

- All release versions of CESM have been updated to run on Derecho (and fix some new github checkout issues). The best option is to update to the newest tag for the release you are using, if possible:
 - <u>CESM 2.1.5</u>
 - <u>CESM 2.2.2</u>
 - <u>CESM 2.3 alpha 17a</u>
- Moving to Derecho or updating will cause answer changes, so proceed carefully. If you do not want to update to one of these tags, contact me (katec@ucar.edu) to discuss other options.



Prompt: A heroic glacier scientist at work, digital art



Python Environments on Derecho

- Casper continues to be available in the same ways as previous, no current timeframe for retirement or replacement
- Python 3.1+ supported module load conda conda activate npl
- CISL python and conda documentation:

https://arc.ucar.edu/knowledge_bas e/83853599

 Jupyterhub can run notebooks on Casper and Derecho

 Fremet: The collest glacier

Prompt: The coolest glacier scientist in town in steampunk style





Diagnostics Updates

- Work on a LIWG diagnostics package goals:
 - A simple to run, but comprehensive view of GrIS and/or AIS over the course of a run
 - A "first-look" package to check for general realism and possible issues as a run proceeds.
 - Model run vs another run or model run vs observations.



- Add option for history output more in-line with CESM as a whole and CMIP requirements, possibly reorganize history and namelists
- Ice-sheet diagnostic notebooks focusing on CISM and coupler output first, other components later.





Prompt: A scientific diagram of the Greenland ice sheet

Diagnostics: CUPiD

- CUPiD: CESM Unified
 Postprocessing and Diagnostics
- <u>https://github.com/NCAR/CUPiD</u>
- Effort currently underway to build a package to support CESM3 evaluation and development in final stages
- Land Ice diagnostics to lean heavily into this framework to reuse building-block code and ensure compatibility across CESM



Prompt: A renaissance painting of scientists working on ice sheets

 Includes integration of the ADF (AMWG Diagnostic Framework) and Ocean model diagnostics



Diagnostics: BATS & LivvKit

- Have ported BATS the Build and Test System - to Derecho
 - <u>https://github.com/Katetc/BATS</u>
 - <u>https://github.com/LIVVkit/BAT</u>
 <u>S</u>
- Will finish this and issue a PR soon
- Next will be port LIVVkit the Land Ice Verification and Validation kit for use with CISM3
- Goal would be to integrate this work into the LIWG diagnostics package as well.



Prompt: A glacier scientist working in watercolor style



Other Projects

- Negative water flux work continues, but lower priority during Derecho launch. Will be finished by CESM3 freeze this summer.
- Ghub project focus this year is on running a simple version of CISM as a "tutorial" on their hosted machines.



Prompt: A glacier scientist as an anime character

- Hopeful to be able to have an interactive model that allows anybody with a free Ghub account to run and learn about CISM.
- Will integrate through the notebook-based tools on Ghub
- Discussions on feasibility look promising and some early work on integration with U Buffalo machines beginning.



Thank you!

Questions, comments, discussion welcome!



Prompt: A heroic glacier scientist saving planet earth



Just for fun



Prompt: An ancient Roman painting of glacier scientists working on ice sheets



Prompt: A black and white studio portrait of a glacier scientist with dramatic backlighting

