

Recommendations for software tools and best practice

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*8th Meteorology Research Away Day, 2024-06-13
Palmer Building, UoR Whiteknights Campus*



**National Centre for
Atmospheric Science**
NATURAL ENVIRONMENT RESEARCH COUNCIL



**University of
Reading**

Recommendations for software tools and best practice

*(+ related topics:
computing, data,
computational
and data-based
work, etc.)*

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1. Tooling: on home turf

- In UoR Meteorology, we have plenty of sub-groups and individuals who develop/maintain, and/or have expertise in, various software tools, processes and best practice
- I'll focus in on myself and the group I am in, as an illustration...

- **NCAS Computational Modelling Services (NCAS-CMS)** “provides computational modelling services *to the UK academic atmospheric and polar science community*” i.e. all of you included. Most of us are based at Reading, hence ‘in-house’ support
- If you use software libraries e.g. for working with and analysing data, do any HPC (read: use supercomputers, such as JASMIN, ARCHER), run or configure models, we can probably advise or help you
- See <https://cms.ncas.ac.uk/>, but come talk to us (plenty of representation here today!)



User Support

CMS provides user support to the UK atmospheric and polar science community through our Helpdesk, FAQs and online Documentation

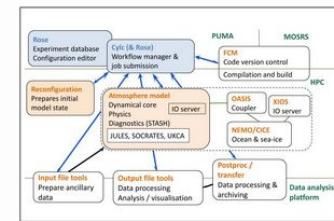
[Learn More >](#)



Services

CMS provides HPC resource management, training and software engineering support for the UK atmospheric and polar science community.

[Learn More >](#)



Infrastructure

CMS provides the infrastructure to allow users to run various complex modelling workflows (e.g. UM, NEMO, etc) on national platforms. We run the PUMA service for access to modelling codes and the Rose/Cylc workflow software.

[Learn More >](#)

1. Tooling: our CF Data Tools

Recipes using cf

Version 3.16.2 for version 1.11 of the CF conventions.

Click on the keywords below to filter the recipes according to their function:

All Aggregate Collapse Contourmap Histogram Lineplot Mathematical Operations Regrid Subspace Mask

cf 3.16.2

A CF-compliant earth science
data analysis library

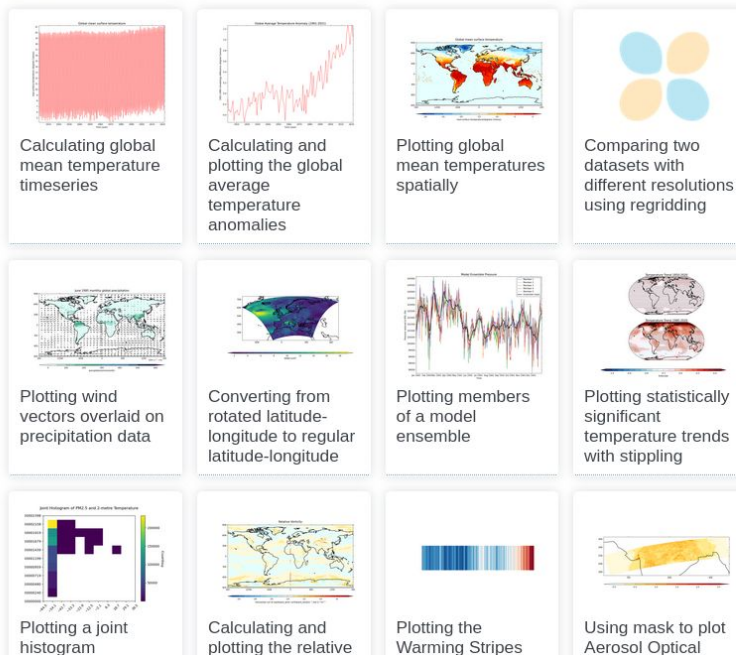
Star 94

Quick search

Go

Introduction
CF data model
Installation
Cheat Sheet
Recipes using cf
Tutorial
Analysis
API reference
Aggregation rules
Performance
Releases
Change log
Contributing

cf development has been
supported by the ERC through
Seachange and Couplet; by the
EC Horizon 2020 programme
through the ENES-1-MERC



- One strand of NCAS-CMS' work is the development of *open-source Python libraries for data analysis, exploration and visualisation of netCDF and Met Office format datasets*, utilising the CF metadata standard to make this simpler and more robust
- If you do that as part of your work, please give these a try:
 - **cf-python** for data analysis
 - <https://ncas-cms.github.io/cf-python/>
 - **cf-plot** for visualisation
 - <https://ncas-cms.github.io/cf-plot/build/>
 - ...**plus other integrated libraries**, see <https://cms.ncas.ac.uk/tools-and-utilities/> for a list with links
- If you need support or would like new features for these, please ask us via contacting by email/message or the Issue Trackers

**Society of Research
Software Engineering**
(UK-based, with international
equivalents)

RSE

"We work to increase software skills across everyone in research, to promote collaboration between researchers and software experts, and to support the creation of an academic career path for Research Software Engineers."



**BETTER
SOFTWARE
BETTER
RESEARCH**

"The first organisation in the world dedicated to improving software in research. It was founded on the premise that helping individuals and institutions understand the vital role that software plays in research would accelerate progress in every field of scientific and academic endeavour."
Motto to the left!

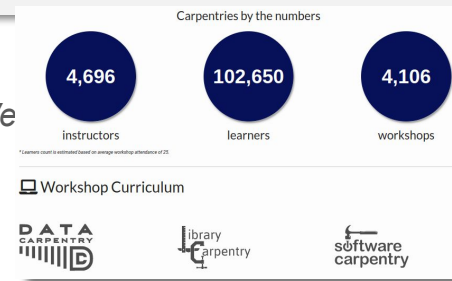
2. Best practice: communities

Examples of **external communities** I advise you check out



The Carpentries

"[We build] global capacity in essential data and computational skills for conducting efficient, open, and reproducible research. We train and foster an active, inclusive, diverse community of learners and instructors that promotes and models the importance of software and data in research."



2. Best practice: standards

Various **standards** have evolved for software/code, data and metadata. We can all work in a consistent and coherent way, maximising interoperability and sharing/reuse potential, if we all abide by these.



Examples are:

1. **Code** standards:

Language-specific style (e.g. PEP8 for Python); design patterns; linting, continuous integration, packaging, documentation infrastructure and structuring, etc.

2. **Data** standards:

Data models; formats (e.g. netCDF); for storage/archiving, discovery and access; use of database & schema; API (application programming interface) design; use of metadata; vocabulary & semantics, etc.

3. **Metadata** standards:

Domain-specific, e.g. CF Conventions for netCDF data, CIM (Common Information Model) for climate models, etc.

Take home points!



If you use or develop software to do, or contribute to, meteorological (or aligned) research, please keep in mind*:

- **In-house expertise, support and software tools (actively-developed) are available.** We're here to help *you* with *your* research, so please make use if you can, submit feature requests if you want more from the tools, etc.
- **There are numerous external (inter)national communities centered around research software** (e.g. improving quality/sustainability, pushing for better recognition of it), both domain-specific and more general. Get involved!
- **Abiding by standards for software/code, data and metadata will make your life easier.**

**and ask us if you want to know more about any of these or have any questions...*