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es-doc for cmip6 (not a summary of es-doc per se)

Bryan Lawrence, Sebastien Denvil, Mark Greenslade, Eric Guilyardi, David Hassell, Sylvia Murphy, Charlotte Pascoe, Allyn Treshansky

The es-doc consortium; IS-ENES2 and NOAA partners

17 February 2016







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| Definition | าร | | | | |

- An experiment is an activity aimed at addressing a specific scientific problem.
- We formally describe such an experiment by means of the NumericalExperiment which describes the experimental aim, and is composed of a set of NumericalRequirements which need to be met to address the experimental aim, these include any spatio-temporal constraints (what domain is simulated, for how long), forcing constraints (e.g. whether a historical or future scenario is used for anthropogenic emissions of radiatively important gases) etc.





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- A Simulation is a run of a configured Model which conforms to the NumericalRequirements, runs on a Platform and produces output Datasets.





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Big Picture Workflow







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| Evolution | | | | | |

- CIM 1.x used for CMIP5; based on XML schema and XML documents produced by the "metafor questionnaire".
 - Limited set of "documents", with much manual work to create model and simulation descriptions)
 - (A document is intended to be a thing created and owned by one entity in the workflow.)





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- Many issues raised with CIM1.x and what we did for CMIP5
- CIM 2.x to be used for CMIP6, based on a completely new method of defining the CIM
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- CIM 2.x to be used for CMIP6, based on a completely new method of defining the CIM
 - ... designed by Mark Greenslade in the toolchain for CMIP5.
- Broad concepts are the same for CMIP6 as CMIP5, but there is more detail.
 - Considerably more "documents", and ways of creating documents.
 - Fixes known problems identified in CIM1.x and addresses community requirements.





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In more detail: CIM2 classes for CMIP6

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CMIP6 Phases and Documents

- Describing the experiments and their requirements so that simulations (and their models) are correctly configured.
- 2 Documenting the actual model configurations used and what scientific processes those models encapsulated.
- 3 Acquiring information about which simulations were run and what data is available.
- Linking simulation information to the various experimental requirements including information about how the simulations might have varied along ensemble axes (conformance).
- **5** Recording the amount of computing used to deliver the experiments (to support assessments of future computing requirements), and
- 6 Documenting the data products themselves.





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Experiment classes







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End-to-End System

- A complete toolchain for producing experiment descriptions via spreadsheets through to display at es-doc.org has been built and exercised (Charlotte and Mark).
- Charlotte is currently fully documenting CMIP6 experiments with the aim to get these included in CMIP6 documentation.
- This all uses an early branch of CIM2, and will be upgraded to the latest version only when it has been completely ratified via the modelling groups - that is, content is dominating over tools ... for experiments, and for now.





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| | es-do | C | Documentation Viewer vo.9.3.1 | ipport | |
| | CMIP6-DRAFT | Experiment : SSP1-26 | i de la constante de la constan | | |
| | Overview | | | | |
| | Project | CMIP6-DRAFT | | | |
| | Name | ssp1-26 | | | |
| | Long Name | SSP1-2.6 | | | |
| | Description | What: SSP-based RCP scenario with low ra RCP2.6 global forcing pathway with SSP1 in 2100. Concentration-driven, Why: The sc The scenario depicts the "best case" future | idiative forcing by the end of the century. Following approximately socioeconomic conditions. Radiative forcing reaches a level of 2.8 enario represents the low end of the range of plausible future pati from the austainability perspective. | W/m2 ways. | |
| | Keywords | Scenario SSP RCP SSP1 RCP2.6 futu | re climate change IPCC ScenarioMIP Low SSP-based RCP | Tier 1 | |
| | Related Experiments | historical | | | |
| | Temporal Constra | ints | | | |
| | 2014/01/01- 2100/01/01 | | | | |
| | Start Date | 2014-01-01 | | | |
| | Required Duration | 86 years | | | |
| | Description | Scenario, from 2014 to the end of the 21st | century. | | |
| | Conformance Requested ? | False | | | |
| | Keywords | future scenario 2014 2100 | | | |
| | Ensemble Require | ements | | | |
| | Historical Initialisation | | | | |
| | Name | HistoricalInitialisation | | | |
| | Description | What: Initialisation is from the end of the Hi the recent past and future scenario simulati | storical experiment. Why: to provide continuity between simulation ons. | is of | |
| | Ensemble Type | Initialisation Method | | | |
| | Minimum Size | 1 | | | |
| | Conformance Requested ? | True | | | |
| | Keywords | initial conditions initialisation historical s | cenario | | |
| | Single Member Ensemb | le | | | |
| | Name | SingleMemberEnsemble | | | |
| | Description | One ensemble member | | | |
| | Ensemble Type | Initialisation | | | |
| | Minimum Size | 1 | | | |
| | Conformance Requested ? | False | | | |
| | Keywords | Single simulation run ensemble | | | |
| | Forcing Constrain | ts | | | |
| | Representative Concent | tration Pathway 2.6 Aerosol Precursor | 3 | | - |
| 📿 /is-en | es Name | RCP26aerpre | | es 🦲 es | s-doc |



Re

Name Description

What: Impose changing concentrations of RCP2.6 aerosol precursors. Why: Represents the low end of the range of plausible future pathways.

Earth System Documentation

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Key changes for describing Configured Models

- CIM2 no longer confuses software components with scientific content (aka components)
- CIM2 is much simpler for describing scientific content, with no capability for infinite nesting.
- Design now aimed at simpler entry via spreadsheets (if desired) and easier configuration of comparison tables (conceptually, the software was already able to cope).
- The old complex vocabularies (not to be confused with lists of terms) are now defined using the same formalism as CIM2 itself (albeit with a shorthand notation).
- Everything can now be versioned and managed in Git





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Scientific Descriptions







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Some Vocabulary Examples





OceanTimesteppingProps

(All these figures autogenerated from the definitions.)





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Most tooling now autogenerated

| Collection | Document | designing | Help |
|--------------|---------------|-----------------------------|-----------|
| Collection - | | planning | Documents |
| ollection d | ocuments for | documenting runs | |
| ensemble | conformance | documenting models other | |
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Developed a GUI desktop tool as part of the design of CIM2, which provides a complete data entry functionality, and can be used for the Milestone 113.

This tool is not intended for primary data entry by modelling groups, who we expect to use other routes, of which more later





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Most tooling now autogenerated

| Collection D | ocument § | designing Help |
|-----------------|------------|------------------------------|
| Collection | | planning Documents |
| Collection docu | ments for | documenting runs |
| ensemble co | informance | documenting models other |
| 0 documents | s; Mode: 💿 | Single Multi |
| | | Documents |
| | | New Conformance New Ensemble |
| | | name |
| | | long_name 🔒 |
| | | description None |
| | | (Responsible_parties None |
| | | (Citation) None |
| | | (Meta) bryan |
| | | (NumericalExperiment) |
| | | UbeEnsemble) None |
| | | Common_conformances |
| 1 | | has_ensemble_axes None |
| atus: New Co | -En | (Ensentablenter) None |
| | | |

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Managing notebook and CIM2

- As of today, the authoritative CIM2 is https://bitbucket.org/bnlawrence/esdoc-nb/.
- It will move to https://github.com/ES-DOC/esdoc-mp/ as soon as is practical (hopefully by, or during the March es-doc sprint.
- At which point I have to stop being in the critical path ...





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Everything else (which is much more)

Sustained effort by Mark Greenslade to ensure that the CIM2 developments will be supportable within the es-doc website and toolchain. Key components will include (but not be limited to):

- 1 esdoc-py-client: python tools for creating and manipulating documents (and other things)
- 2 esdoc-shell: command line shell tools for es-doc
- **3** esdoc-web: software for the esdoc website.
- 4 esdoc-mp: the "canonical" meta-programming framework
- 5 esdoc-api: web service API in support of ES-DOC eco-system
- 6 esdoc-js-client: tool for calling esdoc from javascript
- Also major effort by Allyn Treshansky:
 - esdoc-questionnaire: tooling for creating documents using a traditional questionnaire technique.





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Documents and Status

| Document Family | Creation Tools | Point of Contact | Status |
|-----------------------------|---|-----------------------------------|---|
| Experiments | Spreadsheet, notebook | Charlotte Pascoe | Complete pipeline exists |
| Science | pyesdoc, NOAA questionnaire, (notebook) | Bryan Lawrence (David Hassell) | In development |
| Dataset (inc Simulation) | python parser (in esgf publication workflow) | David Hassell | tested for cmip5 awaiting cmip6 file finalisation |
| Ensemble (further info) | NOAA questionnaire, Spreadsheet | tbd | yet to start tools |
| Party, References | NOAA questionnaire, uploader, (zotero connector?) | tbd | yet to start tools |
| Performance | NOAA questionnaire, spreadsheet, notebook | tbd | yet to start tools |

All documents will be viewable in es-doc.org, although there is a significant amount of work still needed on templates. It will be possible to download tables and documents for use in papers and presentations.





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Timeline for Scientific Vocabularies

| Time line 2016 | Activity or milestone | Owner |
|----------------|---|--------------------|
| By now | Identify experts to produce first version of | Eric and David |
| | realm + WGCM tables | |
| February | Finalise first version of | Charlotte, Bryan, |
| | ocean/seaice/atmosphere + WGCM tables | Eric |
| F2F (March) | Finalise CIM2 and CMIP6 documentation | ES-DOC |
| | workflow | |
| End March | First version of (all) realms and WGCM | Charlotte, Bryan, |
| | tables ready (taking into account inputs from | Eric + experts for |
| | core experts) | other realms |
| April-June | Review of CV.py by modelling groups and | David and Eric |
| | users | |
| End June | CV.py files + es-doc tools (creation and | ES-DOC/WIP |
| | view) ready for wider community testing | |
| July | Release WGCM model tables | ES-DOC/WIP |
| Dec | Release CMIP6 documentation complete | ES-DOC/WIP |
| | procedure for community | |





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Putting it all together

There is a draft WIP paper on this which needs to go onto a public git repository soon.

Issues remain with relationship with internal file metadata in CMIP6 and with the links between content in file and es-doc \ldots .

We have a major sprint/workshop planned for March 8/9/10 in Abingdon, UK, at which point most of the major decisions will be finalised, and we will finalise our plans for IS-ENES2 deliverables and milestones.





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The Future

es-doc relies on key competencies:

- Scientific direction, maintenance, management
- Software leadership, project management, support for developers.
- Software engineering
- Systems
- Support for producers and consumers
- ... but it will have no core funding anywhere after the end of IS-ENES2.





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 - Systems
 - Support for producers and consumers
- ... but it will have no core funding anywhere after the end of IS-ENES2.

Currently implemented in:

- Too few people, who are part-time, and not always able to work on the same things at the same time.
- Too dependent on Bryan and Mark (in different ways).

This is only going to get worse if we can't get

- New funding, that is
- Capable of supporting at least the Bryan and Mark
 functions full time with some backup elsewhere.



