COMMON
WORKFLOW
LANGUAGE

Portable workflow creation and deployment with the CWL standards

Michael R. Crusoe CWL Project Lead
2018-03-07 @biocrusoe / #CommonWL
NITRD MAGIC team meeting

Common Workflow Language v1.0

- Common **declarative** format for tool & workflow execution
- Community based standards effort, not a specific software package; **Very extensible**
- Defined with a schema, specification, & test suite
- Designed for shared-nothing clusters, academic clusters, cloud environments, and local execution
- Supports the use of containers (e.g. Docker) and shared research computing clusters with locally installed software

Why have a standard?

- Standards create a surface for collaboration that promote innovation
- Research frequently dip in and out of different systems but interoperability is not a basic feature.
- Funders, journals, and other sources of incentives prefer standards over proprietary or single-source approaches

Existing computational research workflow systems

1. Arvados http://arvados.org
2. Taverna http://www.taverna.org.uk/
3. Galaxy http://galaxyproject.org/
4. SHIWA https://www.shiwa-workflow.eu/
5. Oozie https://oozie.apache.org/
6. DNANexus https://wiki.dnanexus.com/API-Specification-v1.0.0/IO-and-Run-Specifications# https://wiki.dnanexus.com/API-Specification-v1.0.0/Workflows-and-Analyses#
7. BioDT http://www.biodatomics.com/
8. Agave http://agaveapi.co/live-docs/
9. DiscoveryEnvironment http://www.iplantcollaborative.org/ci/discovery-environment
10. Wings http://www.wings-workflows.org/
11. Knime https://www.knime.org/
12. make, rake, drake, ant, scons & many others. Software development relies heavily on tools to manage workflows related to compiling and packaging applications. For the most part these are file based and usually run on a single node, usually supporting parallel steps (make -j) and in some cases able to dispatch build steps to other machines (https://code.google.com/p/distcc/) https://github.com/Factual/drake
13. Snakemake https://bitbucket.org/snakemake/snakemake
14. BPipe http://bpipe.org
15. Ruffus https://code.google.com/p/ruffus/
16. NextFlow http://nextflow.io
17. Luigi http://github.com/spotify/luigi

Permalink: https://s.apache.org/existing-workflow-systems

Existing computational research workflow systems

18. SciLuigi. Helper library built on top of Luigi to ease development of Scientific workflows in Luigi: http://github.com/samuell/sciluigi
19. GATK Queue https://www.broadinstitute.org/gatk/guide/topic?name=queue
20. Yabi https://ccg.murdoch.edu.au/yabi
21. seqware Workflows are written in Java and executed using the Oozie Workflow Engine on Hadoop or SGE clusters. Uses Zip64 files to group the workflow definition file, workflow itself, sample settings, and data dependencies in a single file that can be exchanged between SeqWare users or archived. https://seqware.github.io/ https://seqware.github.io/docs/6-pipeline/
22. Ketrew https://github.com/hammerlab/ketrew
23. Pegasus http://pegasus.isi.edu/
24. Airflow https://github.com/airbnb/airflow
25. Cosmos https://cosmos.hms.harvard.edu/documentation/index.htmlhttp://bioinformatics.oxfordjournals.org/content/early/2014/07/24/bioinformatics.btu385.full [paper] Cosmos2: https://github.com/LPM-HMS/COSMOS2 http://cosmos.hms.harvard.edu/COSMOS2/
26. Pinball https://github.com/pinterest/pinball
27. bcbio https://bcbio-nextgen.readthedocs.org/en/latest/
28. Chronos https://github.com/mesos/chronos
29. Azkaban https://azkaban.github.io/
30. Apache NiFi https://nifi.apache.org/docs/nifi-docs/html/overview.html
31. flowr (R-based) http://docs.flowr.space/ https://github.com/sahilseth/flowr
32. Mistral https://github.com/arteria-projecthttps://wiki.openstack.org/wiki/Mistral#What_is_Mistral.3Fhttps://wiki.openstack.org/wiki/Mistral/DSLv2
33. nipype http://nipy.org/nipype/
34. End of Day https://github.com/joestubbs/endofday
35. BioDSL https://github.com/maasha/BioDSL
36. BigDataScript http://pcingola.github.io/BigDataScript/
37. Omics Pipe: uses Ruffus http://sulab.scripps.edu/omicspipe/
38. Ensembl Hive https://github.com/Ensembl/ensembl-hive

Existing computational research workflow systems

39. QuickNGS http://bifacility.uni-koeln.de/quickngs/web
40. GenePattern http://www.broadinstitute.org/cancer/software/genepattern/
41. Chipster http://chipster.csc.fi/
42. The Genome Modeling System https://github.com/genome/gms
43. Cuneiform, A Functional Workflow Language https://github.com/joergen7/cuneiformhttp://www.cuneiform-lang.org/
44. Anvaya http://www.ncbi.nlm.nih.gov/pubmed/22809419http://webapp.cabgrid.res.in/biocomp/Anvaya/ANVAYA_Main.html#HOWTO_INSTALL_ANVAYA
45. Makeflow http://ccl.cse.nd.edu/software/makeflow/
46. Airavata http://airavata.apache.org/
47. Pyflow https://github.com/Illumina/pyflow
48. Cluster Flow http://clusterflow.io
49. Unipro UGENE http://ugene.net/ https://dx.doi.org/10.7717/peerj.644
50. CloudSlang http://www.cloudslang.io/
51. Stacks http://catchenlab.life.illinois.edu/stacks/
52. Leaf http://www.francesconapolitano.it/leaf/index.html
53. omictools http://omictools.com/
54. Job Description Language. The Job Description Language, JDL, is a high-level, user-oriented language based on Condor classified advertisements for describing jobs and aggregates of jobs such as Direct Acyclic Graphs and Collections. https://edms.cern.ch/ui/file/590869/1/WMS-JDL.pdf
55. YAWL yet another workflow language http://dx.doi.org/10.1016/j.is.2004.02.002http://www.yawlfoundation.org/
56. Triquetrum https://projects.eclipse.org/projects/technology.triquetrumhttps://github.com/eclipse/triquetrum/
57. Kronos https://github.com/jtaghiyar/kronos
58. qsubsec http://doi.org/10.1093/bioinformatics/btv698 https://github.com/alastair-droop/qsubsec
59. YesWorkflow http://yesworkflow.org
60. GWF - Grid WorkFlow https://github.com/mailund/gwf http://mailund.github.io/gwf/
61. Fireworks https://pythonhosted.org/FireWorks/

Existing computational research workflow systems

62. NGLess: NGS with less work http://ngless.rtfd.io
63. pypipegraph https://github.com/TyberiusPrime/pypipegraph
64. Cromwell https://github.com/broadinstitute/cromwell
65. Dagobah - Simple DAG-based job scheduler in Python. https://github.com/thieman/dagobah
66. sushi https://github.com/uzh/sushi
67. Clinical Trial Processor - A program for processing clinical trials data.http://mircwiki.rsna.org/index.php?title=MIRC_CTP
68. Noodles http://nlesc.github.io/noodles/
69. Swift http://swift-lang.org/main/
70. Consonance (runs SeqWare & CWL) https://github.com/Consonance/consonance/wiki
71. Dog https://github.com/dogtools/dog
72. Produce https://github.com/texttheater/produce
73. LONI Pipeline http://pipeline.loni.usc.edu/
74. Cpipe https://github.com/MelbourneGenomics/cpipe
75. AWE https://github.com/MG-RAST/AWE
76. (Py)COMPSs https://www.bsc.es/research-and-development/software-and-apps/software-list/comp-superscalar/
77. KLIKO https://github.com/gijzelaerr/kliko
78. Script of Scripts https://github.com/BoPeng/SOS http://vatlab.github.io/SOS/
79. XNAT Pipeline Engine https://wiki.xnat.org/display/XNAT/Pipeline+Enginehttps://wiki.xnat.org/display/XNAT/XNAT+Pipeline+Development+Schema
80. Metapipe https://github.com/TorkamaniLab/metapipe
81. OCCAM (Open Curation for Computer Architecture Modeling) https://occam.cs.pitt.edu/
82. Copernicus http://www.copernicus-computing.org
83. iRODS Rule Language https://github.com/samuell/irods-cheatsheets/blob/master/irods-rule-lang-full-guide.md
84. VisTrails https://www.vistrails.org
85. Bionode Watermill https://github.com/bionode/bionode-watermill

Existing computational research workflow systems

86. BIOVIA Pipeline Pilot Overview http://accelrys.com/products/collaborative-science/biovia-pipeline-pilot/
87. Dagman A meta-scheduler for HTCondor https://research.cs.wisc.edu/htcondor/dagman/dagman.html
88. UNICORE https://www.unicore.eu/docstore/workflow-7.6.0/workflow-manual.html#wf_dialect
89. Toil (A scalable, efficient, cross-platform and easy-to-use workflow engine in pure Python) https://github.com/BD2KGenomics/toil
90. Cylc https://cylc.github.io/cylc/
91. Autodesk Cloud Compute Canon https://github.com/Autodesk/cloud-compute-cannon
92. Civet https://github.com/TheJacksonLaboratory/civet
93. Cumulus https://github.com/Kitware/cumulus
94. High-performance integrated virtual environment (HIVE) https://hive.biochemistry.gwu.edu
95. Cloudgene http://cloudgene.uibk.ac.at/cloudgene-yaml
96. FASTR https://bitbucket.org/bigr_erasmusmc/fastr/ http://fastr.readthedocs.io/en/stable/
97. BioMake https://github.com/evoldoers/biomake http://dx.doi.org/10.1101/093245
98. remake https://github.com/richfitz/remake
99. SciFloware http://www-sop.inria.fr/members/Didier.Parigot/pmwiki/Scifloware/
100. OpenAlea http://openalea.gforge.inria.fr/dokuwiki/doku.php https://hal.archives-ouvertes.fr/hal-01166298/file/openalea-PradalCohen-Boulakia.pdf
101. COMBUSTI/O https://github.com/jarlebass/combustio http://hdl.handle.net/10037/9361
102. BioCloud https://github.com/ccwang002/biocloud-server-kaihttp://doi.org/10.6342/NTU201601295
103. Triana http://www.trianacode.org/
104. Kepler https://kepler-project.org/
105. Anduril http://anduril.org/site/
106. dgsh http://www.dmst.aueb.gr/dds/sw/dgsh/
107. EDGE bioinformatics: Empowering the Development of Genomics Expertise https://bioedge.lanl.gov/edge_ui/ http://edge.readthedocs.io/ https://lanl-bioinformatics.github.io/EDGE/
108. Pachyderm http://pachyderm.io/http://pachyderm.readthedocs.io/en/stable/advanced/advanced.html

Existing computational research workflow systems

130. Digdag https://www.digdag.io/
131. Agua / Automated Genomics Utilities Agent http://aguadev.org
132. BioDepot Workflow Builder (BwB) https://github.com/BioDepot/BioDepot-workflow-builderhttps://doi.org/10.1101/099010
133. IMP: a pipeline for reproducible reference-independent integrated metagenomic and metatranscriptomic analyses http://r3lab.uni.lu/web/imp/ https://doi.org/10.1186/s13059-016-1116-8
134. Butler https://github.com/llevar/butler
135. adage / yadage https://github.com/diana-hep/adage https://github.com/diana-hep/yadage
136. HI-WAY: Execution of Scientific Workflows on Hadoop YARN https://github.com/marcbux/Hi-WAYhttps://openproceedings.org/2017/conf/edbt/paper-248.pdf
137. OpenMOLE https://github.com/openmole/openmole https://www.openmole.org/https://doi.org/10.3389/fninf.2017.00021
138. Biopet https://github.com/biopet/biopet
139. Nephele https://nephele.niaid.nih.gov/
140. TOPPAS http://doi.org/10.1021/pr300187f
141. SBpipe https://pdp10.github.io/sbpipe/ https://github.com/pdp10/sbpipehttps://doi.org/10.1186/s12918-017-0423-3
142. Dray http://dray.it/
143. GenomeVIP https://github.com/ding-lab/GenomeVIP https://doi.org/10.1101/gr.211656.116
144. GridSAM https://sourceforge.net/projects/gridsam/
145. Roddy https://github.com/eilslabs/Roddy
146. SciFlo (historical; doesn't seem to be maintained anymore) https://web.archive.org/web/20161118011409/https://sciflo.jpl.nasa.gov/SciFloWiki/FrontPage
147. GNU Guix Workflow Language https://git.roelj.com/guix/gwl.git#gnu-guix-workflow-language-extension https://github.com/UMCUGenetics/guix-workflows/blob/master/umcu/workflows/rnaseq.scm
148. Porcupine https://timvanmourik.github.io/Porcupine/
149. Parsl (a Parallel Scripting Library for Python) http://parsl-project.org
150. ECFLOW (Workflow primarily for Meteorological Applications) https://software.ecmwf.int/wiki/display/ECFLOW/ecflow+home

Existing computational research workflow systems

130. Ophidia http://ophidia.cmcc.it/
131. WebLicht https://weblicht.sfs.uni-tuebingen.de/
132. GATE Cloud https://cloud.gate.ac.uk/
133. SCIPION http://scipion.cnb.csic.es/m/home/ https://github.com/I2PC/scipion/wiki/Creating-a-Protocol
134. Ergatis http://ergatis.sourceforge.net/
135. TIGR "Workflow" https://sourceforge.net/projects/tigr-workflow/ http://tigr-workflow.sourceforge.net/
136. Archivematica https://wiki.archivematica.org/Main_Page (A preservation workflow system that implements the ISO-OAIS standard using gearman/MCP)
137. Martian http://martian-lang.org/about/
138. BioMAJ http://genouest.github.io/biomaj/
139. Conveyor http://conveyor.cebitec.uni-bielefeld.de (retired). https://academic.oup.com/bioinformatics/article/27/7/903/230562/Conveyor-a-workflow-engine-for-bioinformatic
140. Biopipe http://www.biopipe.org (appears to be defunct) https://www.ncbi.nlm.nih.gov/pmc/articles/PMC403782/
141. Wildfire http://wildfire.bii.a-star.edu.sg/ https://bmcbioinformatics.biomedcentral.com/articles/10.1186/1471-2105-6-69
142. BioWBI http://bioinformatics.hsanmartino.it/bits_library/library/00079.pdf
143. BioWMS http://bioinformatics.hsanmartino.it/bits_library/library/00568.pdf
144. BioMoby http://biomoby.open-bio.org/ https://bmcbioinformatics.biomedcentral.com/articles/10.1186/1471-2105-7-523
145. SIBIOS http://ieeexplore.ieee.org/document/1309094/
146. NGSANE https://github.com/BauerLab/ngsane https://academic.oup.com/bioinformatics/article/30/10/1471/266879/NGSANE-a-lightweight-production-informatics
147. Pwrake https://github.com/misshie/Workflows https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3180464/
148. Nesoni https://github.com/Victorian-Bioinformatics-Consortium/nesoni
149. Skam http://skam.sourceforge.net/skam-intro.html
150. TREVA http://bioinformatics.petermac.org/treva/ http://journals.plos.org/plosone/article?id=10.1371/journal.pone.0095217

Existing computational research workflow systems

151. EGene https://www.semanticscholar.org/paper/EGene-a-configurable-pipeline-generation-system-fo-Durham-Kashiwabara/4c0656195b5efcdd3aa7bdcb55fc95a957c150aa https://academic.oup.com/bioinformatics/article/30/18/2659/2475637/EuGene-PP-a-next-generation-automated-annotation
152. WEP https://bioinformatics.cineca.it/wep/ https://bmcbioinformatics.biomedcentral.com/articles/10.1186/1471-2105-14-S7-S11
153. Microbase http://www.microbasecloud.com/
154. e-Science Central http://www.esciencecentral.co.uk/ https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3538293/
155. Cyrille2 https://bmcbioinformatics.biomedcentral.com/articles/10.1186/1471-2105-9-96
156. PaPy https://code.google.com/archive/p/papy/ https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3051902/
157. JobCenter https://github.com/yeastrc/jobcenter https://scfbm.biomedcentral.com/articles/10.1186/1751-0473-7-8
158. CoreFlow https://www.ncbi.nlm.nih.gov/pubmed/24503186
159. dynamic-pipeline https://code.google.com/archive/p/dynamic-pipeline/
160. XiP http://xip.hgc.jp/wiki/en/Main_Page https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3530915/
161. Eoulsan http://www.outils.genomique.biologie.ens.fr/eoulsan/ https://www.ncbi.nlm.nih.gov/pubmed/22492314
162. CloudDOE http://clouddoe.iis.sinica.edu.tw/
163. BioPig https://github.com/JGI-Bioinformatics/biopig https://www.ncbi.nlm.nih.gov/pubmed/24021384
164. SeqPig https://github.com/HadoopGenomics/SeqPig https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3866557/
165. zymake http://www-personal.umich.edu/~ebreck/code/zymake/
166. JMS https://github.com/RUBi-ZA/JMS http://journals.plos.org/plosone/article?id=10.1371/journal.pone.0134273
167. CLC Genomics Workbench https://www.qiagenbioinformatics.com/products/clc-genomics-workbench/
168. NG6 http://ng6.toulouse.inra.fr/ https://www.ncbi.nlm.nih.gov/pubmed/22958229
169. VIBE http://www.incogen.com/vibe/
170. WDL (Workflow Description Language) https://github.com/broadinstitute/wdl

Existing computational research workflow systems

171. SciFlow https://github.com/kaizhang/SciFlow (not to be confused with SciFloware and SciFlo).
172. Bioshake https://github.com/PapenfussLab/bioshake
173. SciPipe http://scipipe.org
174. Kapacitor / TICKscripts https://docs.influxdata.com/kapacitor/v1.3//tick/
175. AiiDA: Automated Interactive Infrastructure and Database for Computational Science http://www.aiida.net/
176. Reflow: a language and runtime for distributed, integrated data processing in the cloud https://github.com/grailbio/reflow
177. Resolwe: an open source dataflow package for Django framework https://github.com/genialis/resolwe
178. Yahoo! Pipes (historical) https://en.wikipedia.org/wiki/Yahoo!_Pipes
179. Walrus https://github.com/fjukstad/walrus
180. Apache Beam https://beam.apache.org/
181. CLOSHA https://closha.kobic.re.kr/ https://www.bioexpress.re.kr/go_tutorialhttp://docplayer.net/19700397-Closha-manual-ver1-1-kobic-korean-bioinformation-center-kogun82-kribb-re-kr-2016-05-08-bioinformatics-workflow-management-system-in-bio-express.html
182. WopMars https://github.com/aitgon/wopmars http://wopmars.readthedocs.io/
183. flowing-clj https://github.com/stain/flowing-clj
184. Plumbing and Graph https://github.com/plumatic/plumbing
185. LabView http://www.ni.com/en-us/shop/labview.html
186. MyOpenLab http://myopenlab.org/
187. Max/MSP https://cycling74.com/products/max/
188. NoFlo https://noflojs.org/
189. Flowstone http://www.dsprobotics.com/flowstone.html
190. HyperLoom https://code.it4i.cz/ADAS/loom https://code.it4i.cz/ADAS/loom
191. Dask http://dask.pydata.org/en/latest/ https://github.com/dask/dask

Existing computational research workflow systems

193. Stimela https://github.com/SpheMakh/Stimela https://github.com/SpheMakh/Stimela/wiki https://www.acru.ukzn.ac.za/~cosmosafari2017/wp-content/uploads/2017/02/makhathini.pdf
194. JTracker http://www.jthub.co/ https://github.com/icgc-dcc/jtracker
195. PipelineDog http://pipeline.dog/ https://github.com/zhouanbo/pipelinedog https://doi.org/10.1093/bioinformatics/btx759
196. DALiuGE https://arxiv.org/abs/1702.07617 https://github.com/ICRAR/daliuge https://daliuge.readthedocs.io/
197. Overseer https://github.com/framed-data/overseer
198. Squonk https://squonk.it/
199. GC3Pie https://github.com/uzh/gc3pie
200. Fractalide https://github.com/fractalide/fractalide

Permalink: https://s.apache.org/existing-workflow-systems

EBI's metagenomics workflow scripts -> CWL

https://www.ebi.ac.uk/metagenomics/pipelines/3.0

9522 lines of Python, BASH, and Perl code (data analysis workflows logic mixed with operational details

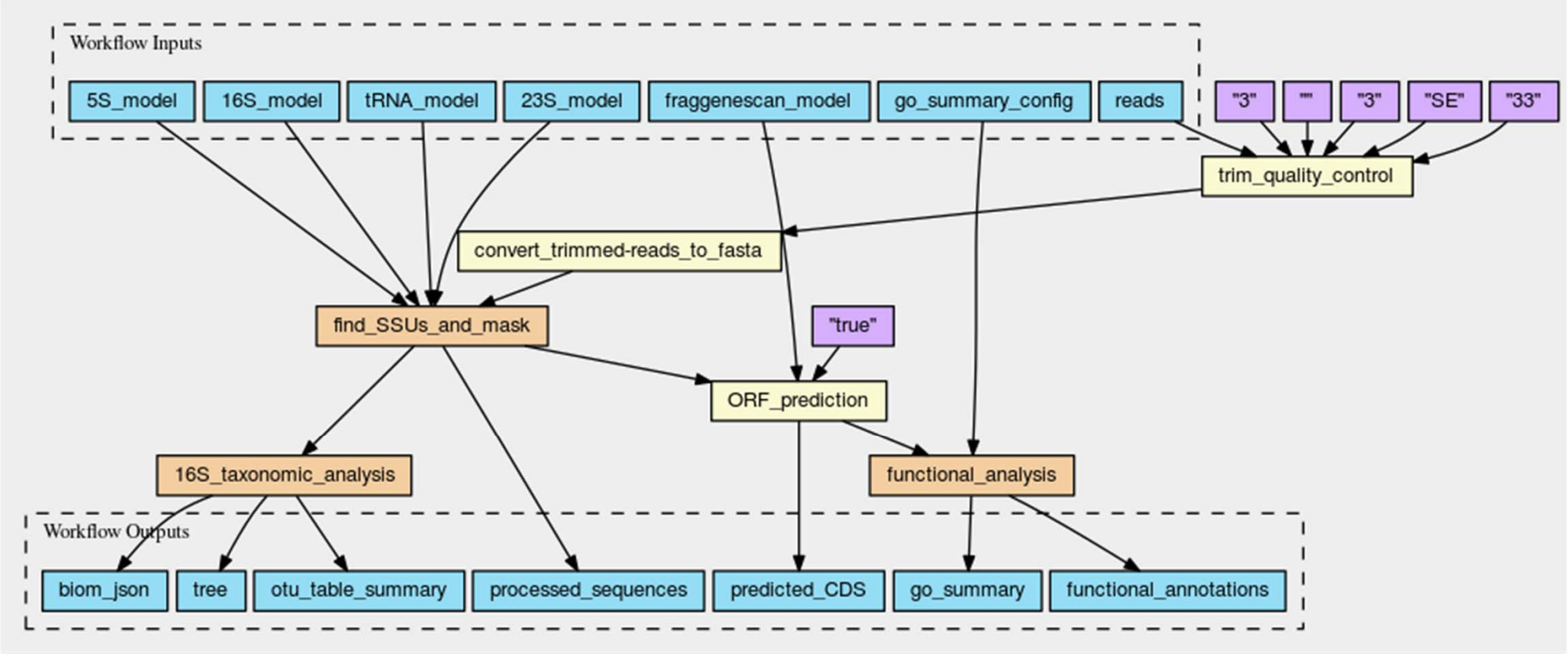
converted into

2560 lines of CWL descriptions

https://github.com/ProteinsWebTeam/ebi-metagenomics-cwl

(Lines of code counts via https://github.com/AlDanial/cloc#Stable)

EBI's metagenomics -> CWL project



Courtesy EMBL-EBI Metagenomics, visualization from

https://view.commonwl.org/workflows/github.com/ProteinsWebTeam/ebi-metagenomics-cwl/blob/master/workflows/rna-selector.cwl

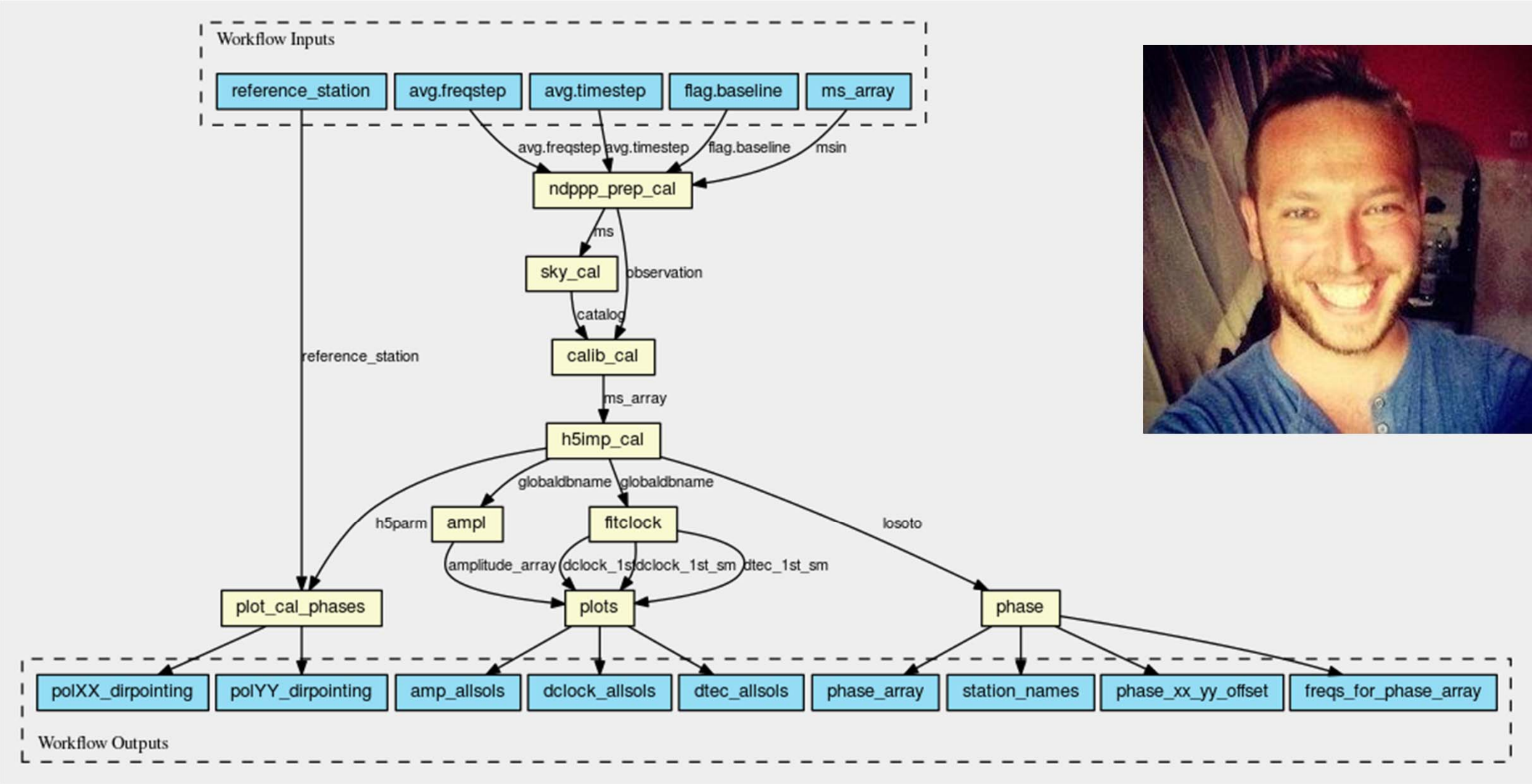
The LOFAR pre-facet calibration pipeline

LOFAR pipelines currently written in ‘parsets’ language **unique to that team**

Gijs Molenaar packaged the software in the KERN suite (3rd party software packages for Ubuntu Linux LTS) and used those packages to create Docker/Singularity containers

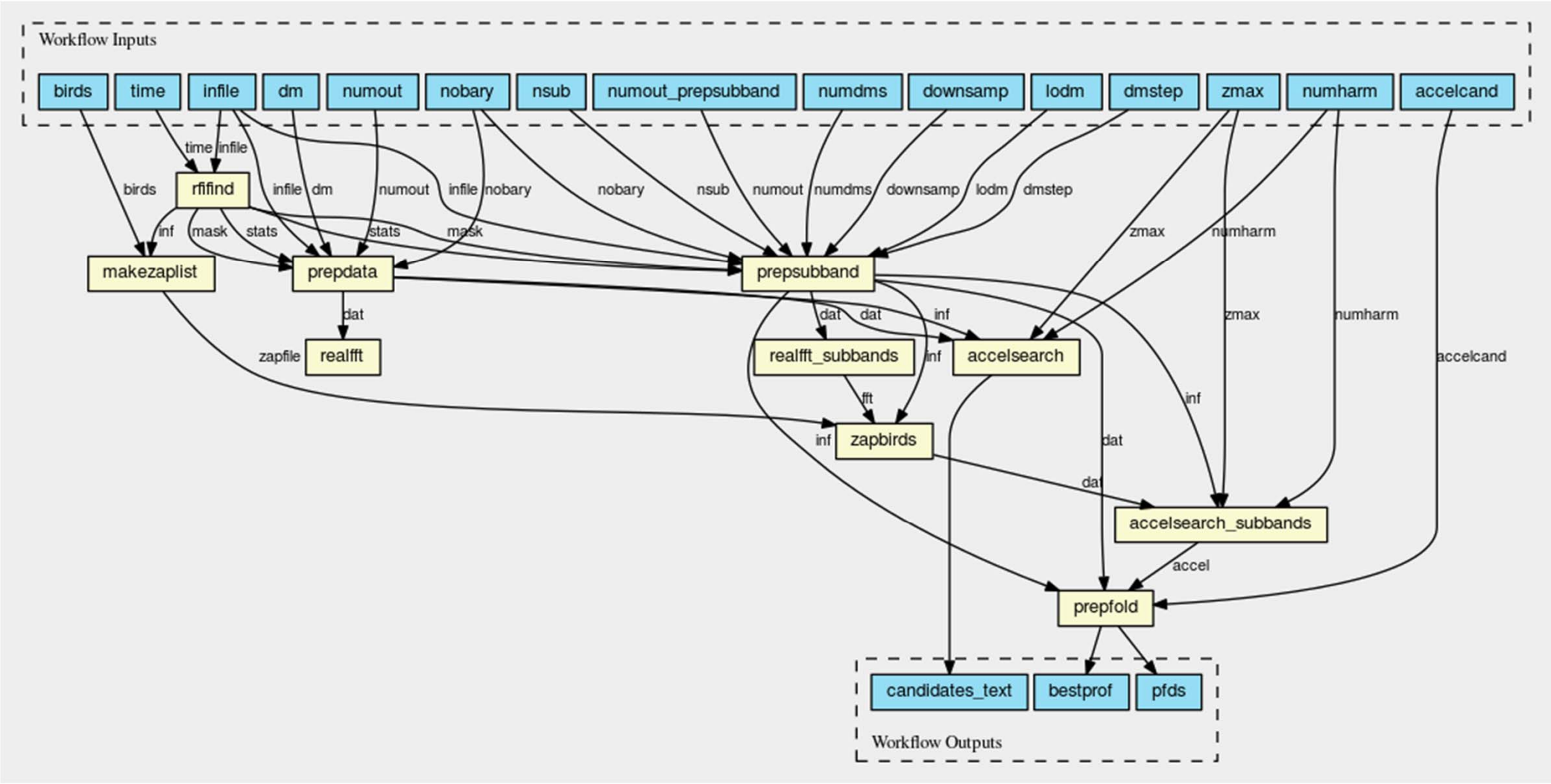
Gijs (with some assistance from me) then converted the “parset” based pipeline to a Common Workflow Language version

The LOFAR pre-facet calibration pipeline



https://view.commonwl.org/workflows/github.com/EOSC-LOFAR/prefactor-cwl/blob/63fcfba8e17a18343eede9cc3bf1c81a10dc2dcc/prefactor.cwl

Searching for Pulsars with PRESTO (& CWL)



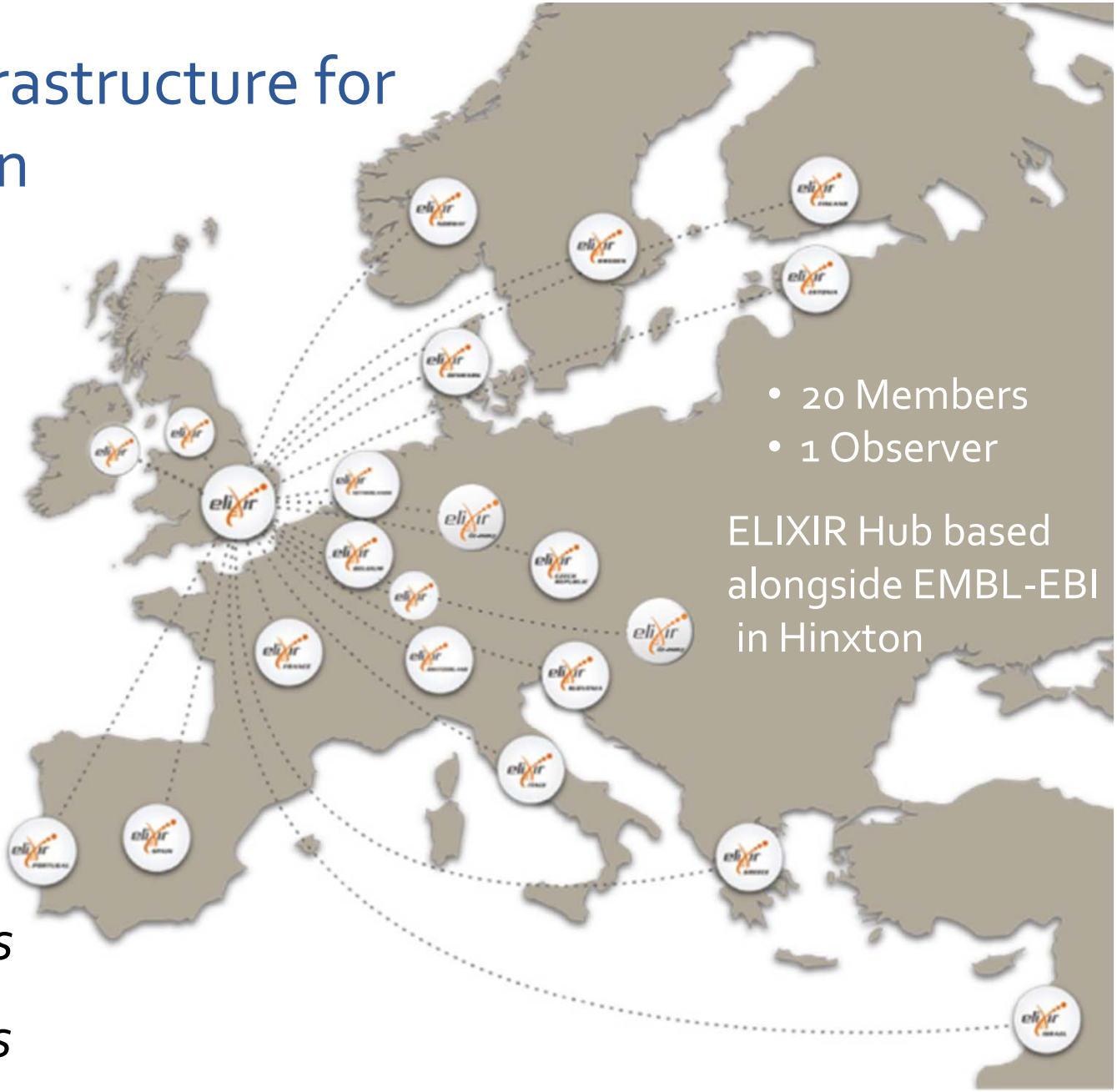
https://view.commonwl.org/workflows/github.com/EOSC-LOFAR/prefactor-cwl/blob/63fcfba8e17a18343eede9cc3bf1c81a10dc2dcc/prefactor.cwl (in progress)

From the Life Sciences…

ELIXIR: European infrastructure for biological information

Data infrastructure for Europe's life-science research:

- *Data*
- *Interoperability*
- *Tools*
- *Compute*
- *Training*



- 20 Members
- 1 Observer

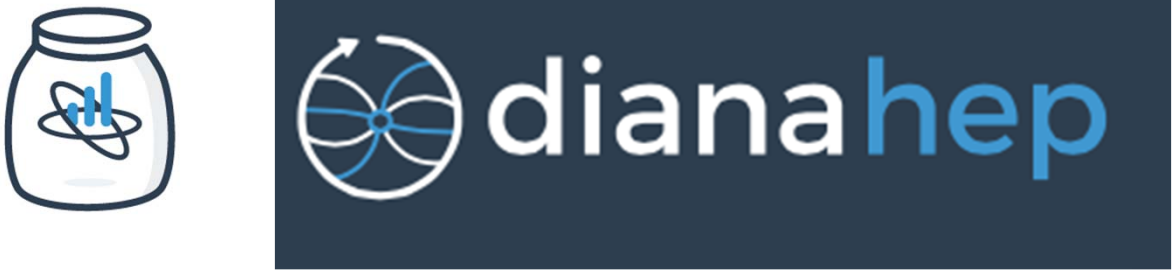
ELIXIR Hub based alongside EMBL-EBI in Hinxton

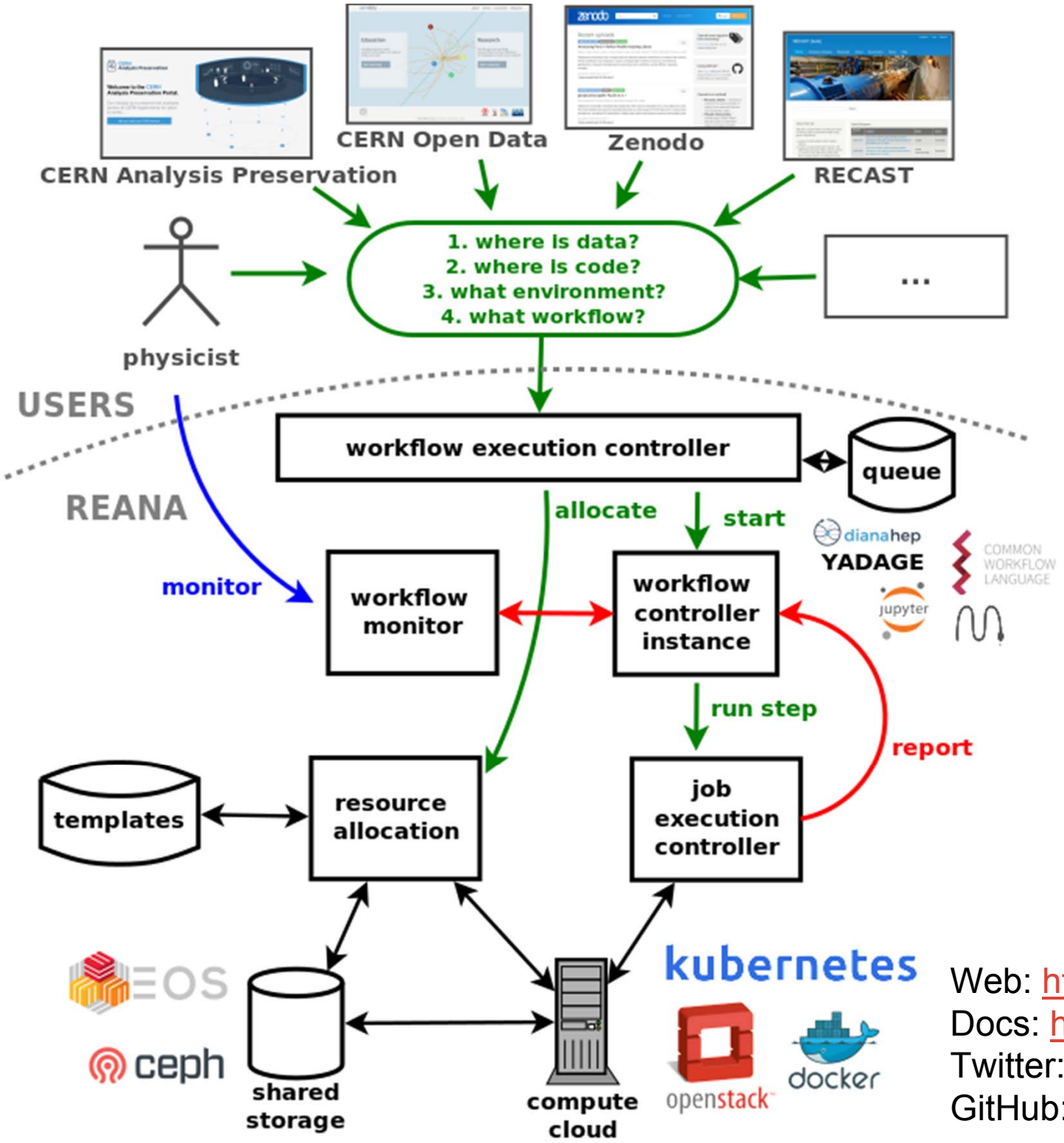
- *Marine metagenomics*
- *Crop and forest plants*
- *Human data*
- *Rare diseases*

www.elixir-europe.org

@ELIXIREurope

…to (astro)physics and beyond





Web: http://reana.io
Docs: http://reana.readthedocs.io
Twitter: https://twitter.com/reanahub
GitHub: https://github.com/reanahub

The CWL model

CWL tool descriptions turn POSIX† command-line data analysis tools into functions

- well defined and named inputs & outputs
- typed

These inputs and outputs are connected into “data flow” style workflows

†The reference CWL runner runs on Microsoft Windows using Docker software containers

Well described workflows → Save time, money

CWL tool descriptions can self describe the “shape” of the computation

- # of cores
- memory needs
- temporary and output storage estimations

This uses fixed values, or can be computed prior to scheduling based upon the input data & its metadata

http://www.commonwl.org/v1.0/CommandLineTool.html#Runtime_environment

Data locality with CWL

Input and output files are modeled in CWL as rich object with identifier (URI/IRI) and other metadata.

Platforms that understand CWL can use these identifiers to send compute to where or near the location of data.

In combination with the resource matchmaking this can conversely result in data being sent to specialized compute as configured by the operator (or machine learning)

Community Based Standards development

Different model than traditional nation-based or regulatory approach

We adopted the Open-Stand.org Modern Paradigm for Standards: Cooperation, Adherence to Principles (Due process, Broad consensus, Transparency, Balance, Openness), Collective Empowerment, (Free) Availability, Voluntary Adoption

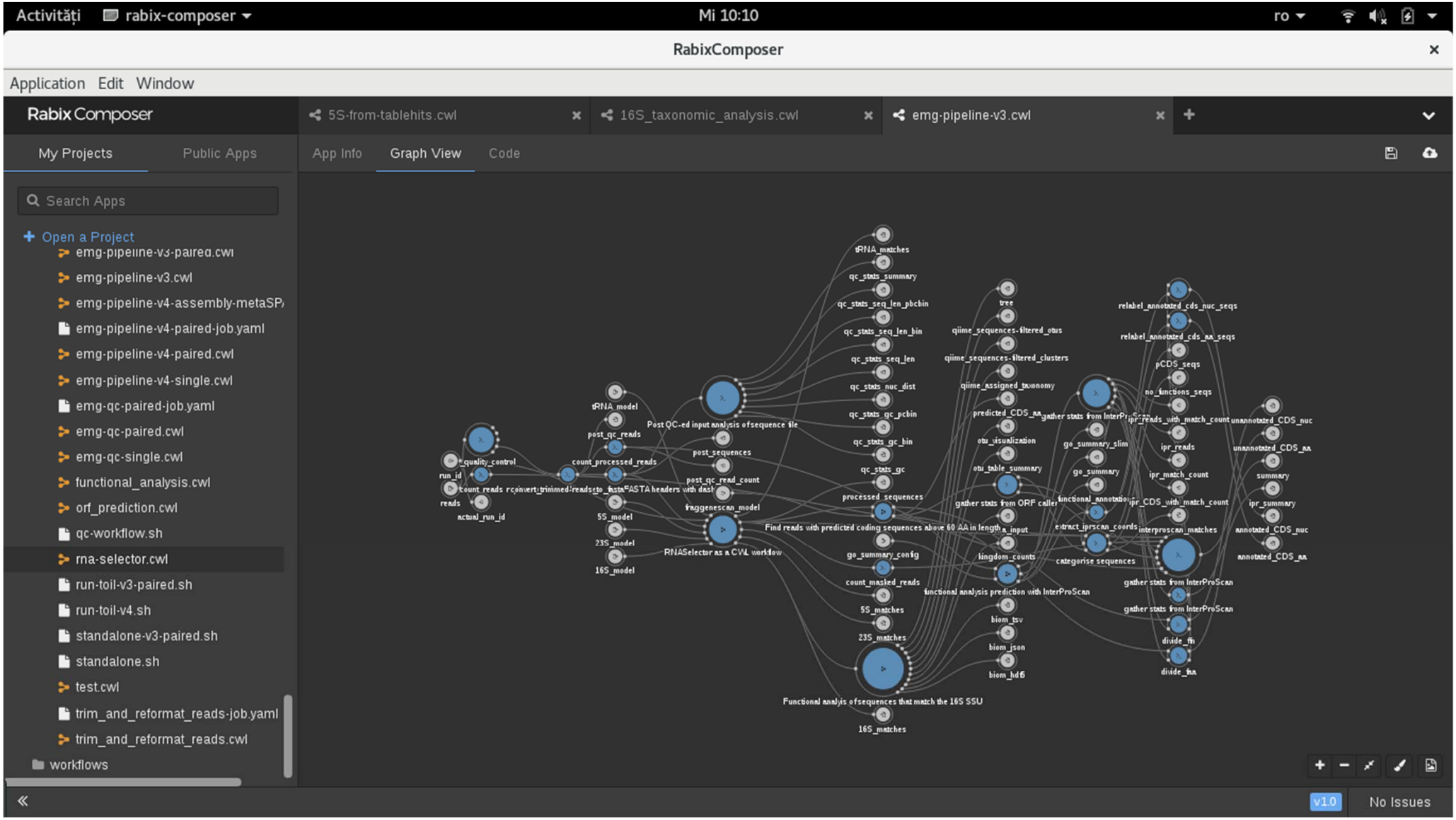
Why use the Common Workflow Language?

Develop your pipeline on your local computer (optionally with software containers)

Execute on your research cluster or in the cloud

Deliver to users via workbenches like Arvados, Rabix, Toil. Galaxy, Apache Taverna, AWE, Funnel (GCP) support is in alpha stage.

Rabix Composer: an Open Source GUI for CWL



Software Containers & CWL

CWL v1.0.x has built in (optional) support for Docker software containers. The CWL reference runner has support for running Docker containers using the Docker, Singularity, uDocker, or dx-docker runtimes.

CWL descriptions can also contain more generic software requirements; can be used to make applications available using Docker, Singularity, conda, Debian, or any other packaging system (like **CVMFS**).

http://www.commonwl.org/v1.0/CommandLineTool.html#SoftwareRequirement

Example with reference CWL runner: https://github.com/common-workflow-language/cwltool#leveraging-softwarerequirements-beta

Software Containers & CWL

Future version of the CWL standard will switch from “Docker” image format for software containers to the Open Container Initiative image format standard.

Recent developments

IBM Spectrum Computing is adding native CWL support to LSF in by the end of Q2

The Toil workflow system has gained HTCondor support

CWL 1.1 will also be release by end of Q2

Key Points

CWL, as a standard, allows us to move the interface between the researcher and the infrastructure to a much higher layer. **This frees the researcher to focus on their work and frees the e-infra providers to better optimize and balance their systems.**

This workflow standard already has a **growing ecosystem**: training materials (in three languages), visualizers, support for popular text editors and IDEs, standalone GUI, and more

Thanks!

http://www.commonwl.org

Backup slides!

Other Early Adopters include

(US) **National Cancer Institute Cloud Pilots** (Seven Bridges Genomics, Institute for Systems Biology)

Cincinnati Children's Hospital Medical Research Center (Andrey Kartashov & Artem Barski)

bcbio: Validated, scalable, community developed variant calling, RNA-seq and small RNA analysis (docs, BOSC 2016 talk: video, slides) (Brad Chapman et al.)

Duke University, Center for Genomic and Computational Biology: **GENOMICS OF GENE REGULATION** project (BOSC 2016 talk: video, slides, poster)(Dan Leehr et al.)

NCI **DREAM SMC-RNA Challenge** (Kyle Ellrott et al.) Presentation ; GA4GH Workflow Execution DREAM Challenge

Funding

Currently, only one FTE! (M. Crusoe). Lots of in-kind donations from participant projects & vendors.

NGO/charity in the USA is legal home of the project (Software Freedom Conservancy, a 501(c)(3))

M. Crusoe recently formed a public enterprise in Lithuania (VšĮ "Darbo eigos") to assist with coordinating & funding CWL work in Europe.

CWL is a standards community & pan-discipline; most traditional funding sources don’t know what to do with us.

Michael R. Crusoe, who is this guy?

From Phoenix, Arizona (Sonoran Desert), USA

Studied at Arizona State: Comp. Sci.; time in industry as a developer & system administrator (Google, others); returned to ASU for B.S. in Microbiology.

Introduced to bioinformatics via Anolis (lizard) genome assembly and analysis (Kenro Kusumi, Arizona State)

Returned to software engineering as a Research Software Engineer for k-h-mer project (C. Titus Brown, Michigan State, then U. of California, Davis)

Now based out of
Vilnius, Lithuania

Assisting EOSCPilot:
LOFAR & eWaterCycle SD

Example: samtools-sort.cwl

File type & metadata

```
class: CommandLineTool
cwlVersion: v1.0
doc: Sort by chromosomal coordinates
```

Runtime environment

```
hints:
  DockerRequirement:
    dockerPull: quay.io/cancercollaboratory/dockstore-tool-samtools-sort
```

Input parameters

```
inputs:
  aligned_sequences:
    type: File
    format: edam:format_2572  # BAM binary alignment format
    inputBinding:
      position: 1
```

Executable

```
baseCommand: [samtools, sort]
```

Output parameters

```
outputs:
  sorted_aligned_sequences:
    type: stdout
    format: edam:format_2572
```

Linked data support

```
$namespaces: { edam: "http://edamontology.org/" }
$schemas: [ "http://edamontology.org/EDAM_1.15.owl" ]
```

File type & metadata

```
class: CommandLineTool
cwlVersion: v1.0
doc: Sort by chromosomal coordinates
```

- Identify as a CommandLineTool object
- Core spec includes simple comments
- Metadata about tool extensible to arbitrary RDF vocabularies, e.g.
  - Biotools & EDAM
  - Dublin Core Terms (DCT)
  - Description of a Project (DOAP)
- GA4GH Tool Registry project will develop best practices for metadata & attribution

Runtime Environment

```
hints:
  DockerRequirement:
    dockerPull: quay.io/[…]samtools-sort
```

- Define the execution environment of the tool
- “requirements” must be fulfilled or an error
- “hints” are soft requirements (express preference but not an error if not satisfied)
- Also used to enable optional CWL features
  - Mechanism for defining extensions

Input parameters

```
inputs:
  aligned_sequences:
    type: File
    format: edam:format_2572  # BAM binary format
    inputBinding:
      position: 1
```

- Specify name & type of input parameters
  - Based on the Apache Avro type system
  - null, boolean, int, string, float, array, record
  - File formats can be IANA Media/MIME types, or from domain specific ontologies, like EDAM for bioinformatics
- “inputBinding”: describes how to turn parameter value into actual command line argument

Example: samtools-sort.cwl

File type & metadata

```
class: CommandLineTool
cwlVersion: v1.0
doc: Sort by chromosomal coordinates
```

Runtime environment

```
hints:
  DockerRequirement:
    dockerPull: quay.io/cancercollaboratory/dockstore-tool-samtools-sort
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Input parameters

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inputs:
  aligned_sequences:
    type: File
    format: edam:format_2572  # BAM binary alignment format
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Executable

```
baseCommand: [samtools, sort]
```

Output parameters

```
outputs:
  sorted_aligned_sequences:
    type: stdout
    format: edam:format_2572
```

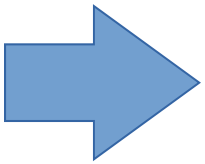
Linked data support

```
$namespaces: { edam: "http://edamontology.org/" }
$schemas: [ "http://edamontology.org/EDAM_1.15.owl" ]
```

Command Line Building

Input object

```
aligned_sequences:
  class: File
  location: example.bam
  format: http://edamontology.org/format_2572
```



```
inputs:
  aligned_sequences:
    type: File
    format: edam:format_2572
    inputBinding:
      position: 1
```

```
baseCommand: [samtools, sort]
```

- Associate input values with parameters
- Apply input bindings to generate strings
- Sort by “position”
- Prefix “base command”

[“samtools”, “sort”, “example.bam”]

Output parameters

```
outputs:
  sorted_aligned_sequences:
    type: stdout
    format: edam:format_2572
```

- Specify name & type of output parameters
- In this example, capture the STDOUT stream from "samtools sort" and tag it as being BAM formatted.

Workflows

- Specify data dependencies between steps
- Scatter/gather on steps
- Can nest workflows in steps
- Still working on:
- Conditionals & looping

Example: grep & count

```
class: Workflow
cwlVersion: v1.0
```

```
requirements:
  - class: ScatterFeatureRequirement
```

```
inputs:
  pattern: string
  infiles: File[]
```

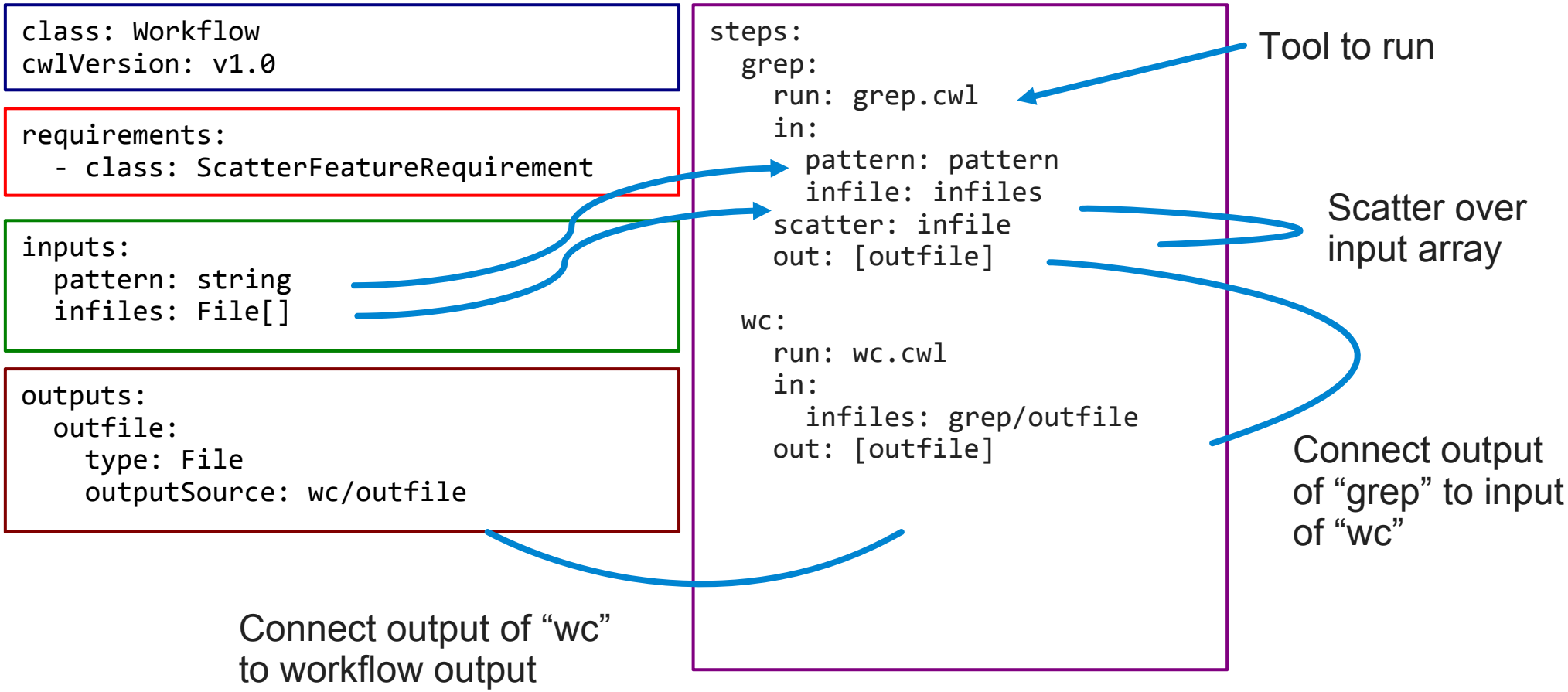
```
outputs:
  outfile:
    type: File
    outputSource: wc/outfile
```

```
steps:
  grep:
    run: grep.cwl
    in:
      pattern: pattern
      infile: infiles
    scatter: infile
    out: [outfile]

  wc:
    run: wc.cwl
    in:
      infiles: grep/outfile
    out: [outfile]
```

Source file: https://github.com/common-workflow-language/workflows/blob/2855f2c3ea875128ff62101295897d8d11d99b94/workflows/presentation-demo/grep-and-count.cwl

Example: grep & count



Use Cases for the CWL standards

Publication reproducibility, reusability

Workflow creation & improvement across institutions and continents

Contests & challenges

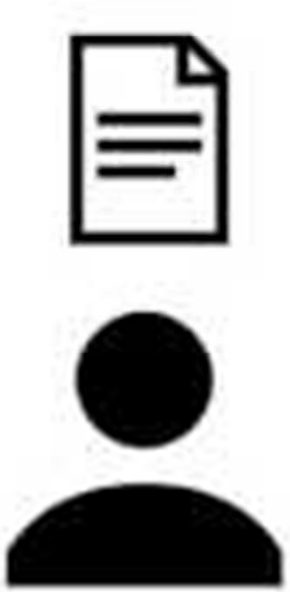
Analysis on non-public data sets, possibly using GA4GH job & workflow submission API

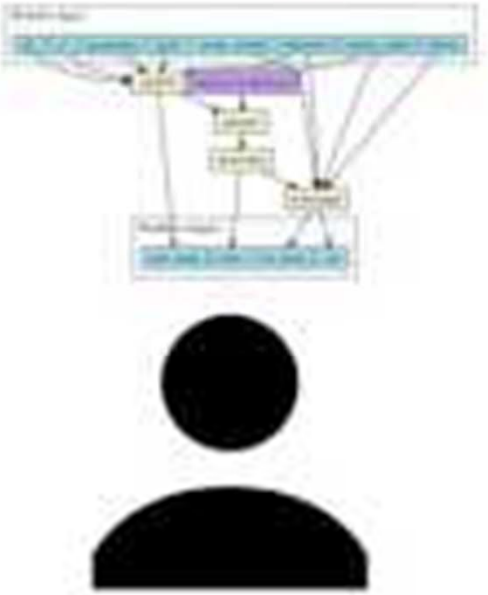
Linked Data & CWL

- Hyperlinks are common currency
- Bring your own RDF ontologies for metadata
- Supports SPARQL to query

Example: can use the EDAM ontology (ELIXIR-DK) to specify file formats and reason about them:

“FASTQ Sanger” encoding is a type of FASTQ file

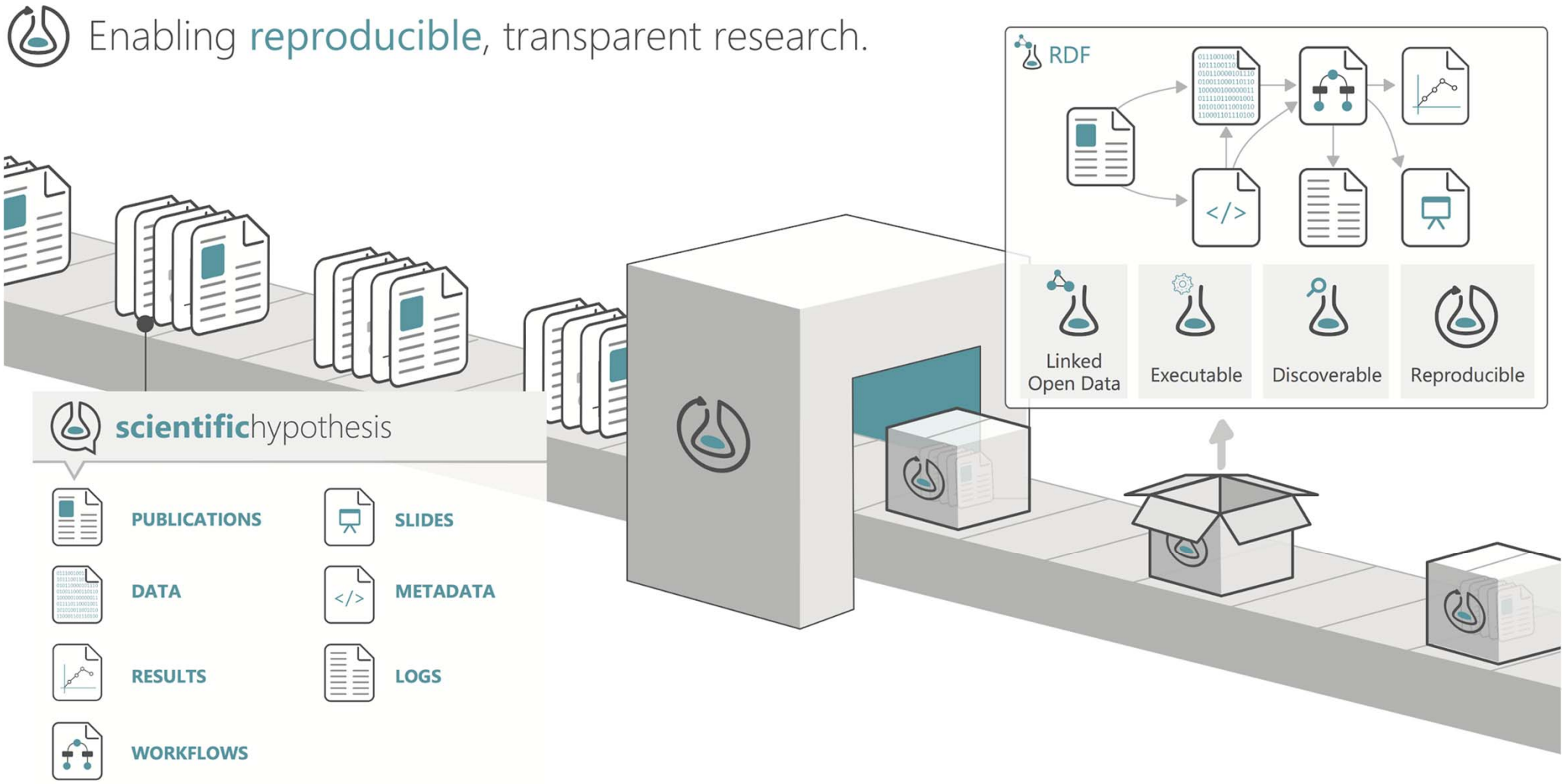




CWL Design principles

- Low barrier to entry for implementers
- Support tooling such as generators, GUIs, converters
- Allow extensions, but must be well marked
- Be part of linked data ecosystem
- Be pragmatic

ResearchObject.org standard overview



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