https://goo.gl/4peVam

COMMON WORKFLOW LANGUAGE

Reproducible Research Data Analysis with the Common Workflow Language standards

Michael R. Crusoe CWL Project Lead
2017-10-02 @biocrusoe / #CommonWL
CERN Computing Seminars and Colloquia

Michael R. Crusoe, who is this guy?

https://goo.gl/4peVam

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 & received B.S. in Microbiology.

Co-author of an identity card **standard** for use by seafarers; accompanying ILO convention ratified by 30+ countries

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)

"Workflows"

We use the word "workflows" as a shorthand for:

the collection of computer applications, scripts, and code used in **computational data analysis**

- how the applications are configured
- and how the data flows between them

(primarily in a research/scientific context)

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Why use a workflow management system?

Features **can** include:

separation of concerns: focus on the science being done first; then optimize execution later
automatic job execution: start a complicated analysis involving many pieces with a single command
scaling (across nodes, clusters, and possibly continents)
automatically generated graphical user interfaces (example: Galaxy)
How was this file made? (**automatic provenance tracking**)

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EBI's metagenomics workflow -> 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)

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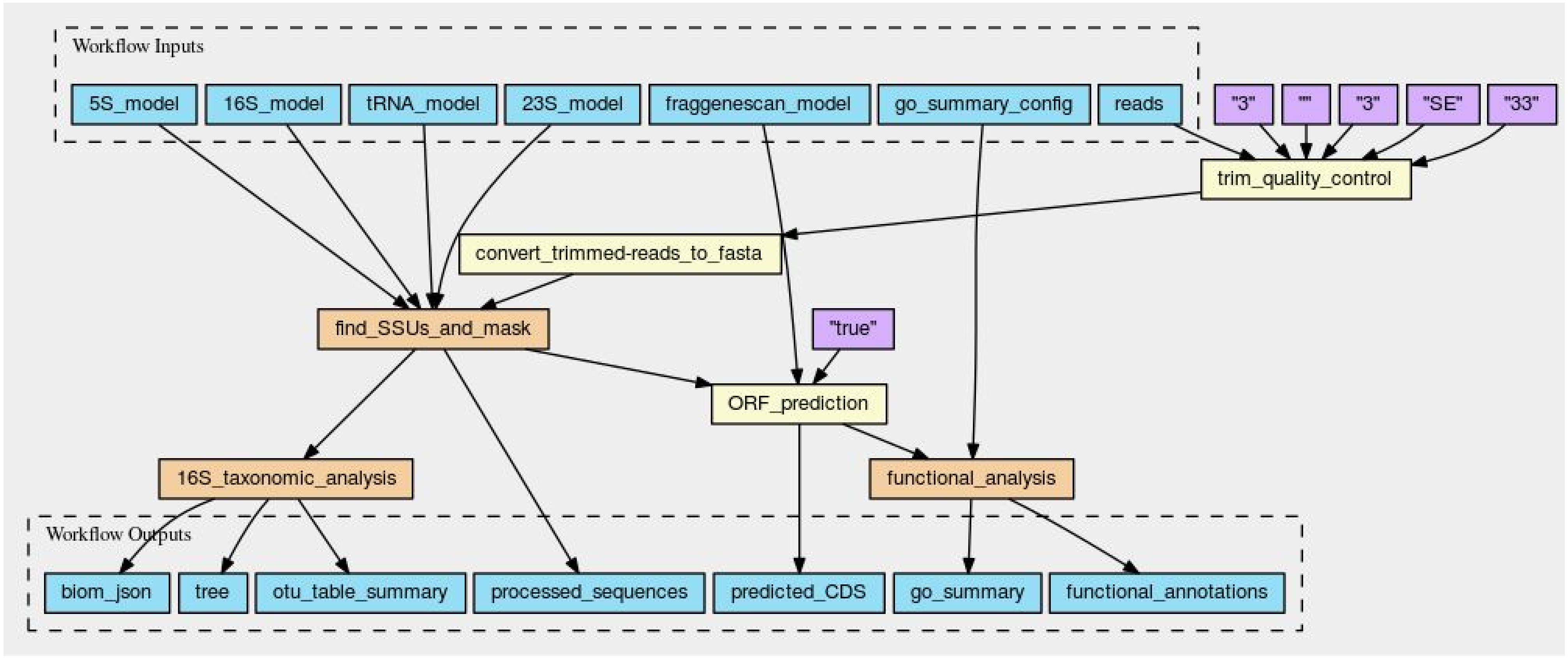
EBI's metagenomics -> CWL project



Courtesy EMBL-EBI Metagenomics, visualization from

https://view.commonwl.org/workflows/github.com/ProteinsWebTeam/ebi-metagenomics-cwl/tree/ca6ca61/workflows/emg-pipeline-v3.cwl

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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

https://github.com/common-workflow-language/common-workflow-language/wiki/Existing-Workflow-systems

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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

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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

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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

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Existing computational research workflow systems

109. Digdag https://www.digdag.io/
110. Agua / Automated Genomics Utilities Agent http://aguadev.org
111. BioDepot Workflow Builder (BwB) https://github.com/BioDepot/BioDepot-workflow-builderhttps://doi.org/10.1101/099010
112. 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
113. Butler https://github.com/llevar/butler
114. adage / yadage https://github.com/diana-hep/adage https://github.com/diana-hep/yadage
115. HI-WAY: Execution of Scientific Workflows on Hadoop YARN https://github.com/marcbux/Hi-WAYhttps://openproceedings.org/2017/conf/edbt/paper-248.pdf
116. OpenMOLE https://github.com/openmole/openmole https://www.openmole.org/https://doi.org/10.3389/fninf.2017.00021
117. Biopet https://github.com/biopet/biopet
118. Nephele https://nephele.niaid.nih.gov/
119. TOPPAS http://doi.org/10.1021/pr300187f
120. SBpipe https://pdp10.github.io/sbpipe/ https://github.com/pdp10/sbpipehttps://doi.org/10.1186/s12918-017-0423-3
121. Dray http://dray.it/
122. GenomeVIP https://github.com/ding-lab/GenomeVIP https://doi.org/10.1101/gr.211656.116
123. GridSAM https://sourceforge.net/projects/gridsam/
124. Roddy https://github.com/eilslabs/Roddy
125. SciFlo (historical; doesn't seem to be maintained anymore) https://web.archive.org/web/20161118011409/https://sciflo.jpl.nasa.gov/SciFloWiki/FrontPage

https://github.com/common-workflow-language/common-workflow-language/wiki/Existing-Workflow-systems

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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

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Common Workflow Language v1.0

- Common 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

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Participating Organizations & Projects

CUROVERSE™

Galaxy PROJECT

SevenBridges genomics

Workflow 4Ever

Taverna

Institut Pasteur

elixir

HARVARD T.H. CHAN SCHOOL OF PUBLIC HEALTH

Cincinnati Children's®

BROA INSTIT

UCSC

The Agave Platform

CYVERSE™

TACC

OHSU

netherlands eScience center

wellcome trust sanger institute

ASTRON

bioexcel

How did we do it?

Initial group started at BOSC Codefest 2014

Moved to open mailing list and extended onto GitHub & then Gitter chat

Frequent (twice a month or more) video chats to work through design issues with summaries emailed

Some participants doing CWL community work during their day jobs, some on “nights & weekends”.

In October 2015 Seven Bridges sponsored one of the co-founders (M. Crusoe) to work full time on the project

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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

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Why use the Common Workflow Language?

Develop your pipeline on your local computer (optionally with 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.

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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

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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

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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

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

```
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  DockerRequirement:
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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" ]
```

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[]
```

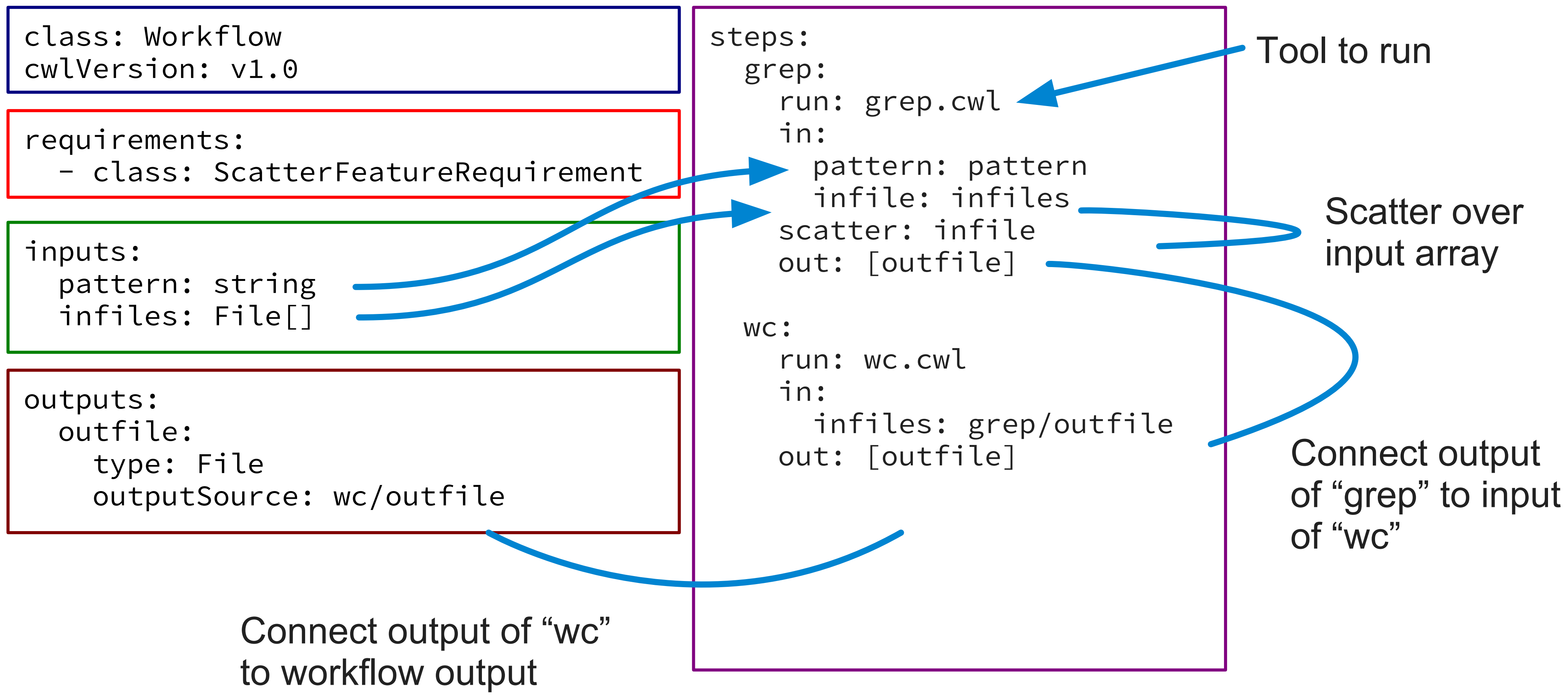
```
outputs:
  outfile:
    type: File
    outputSource: wc/outfile
```

```
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



```
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]
```

Tool to run

Scatter over input array

Connect output of “grep” to input of “wc”

Connect output of “wc” to workflow output

Challenges

Giving a standard to a community that is “free as in puppies”: How does the community participate? How will maintenance be funded?

CWL isn’t the only effort that has these needs; can we join with related efforts?

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A Grand Opportunity

if:

properly funded and embraced by the wider community

then:

the researchobject.org standards + CWL could fulfill the huge need for an executable and complete description of how computationaly derived research results were made

researchobject.org

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What's next for the Common Workflow Language?

Public charity to own the standard

Tooling improvements

More implementations (Galaxy, Taverna, Kepler, Xenon, …?)

Integration with researchobject.org standards for attribution, provenance, and metadata guidance.

Thanks!

http://commonwl.org

https://goo.gl/4peVam

Other Early Adopters

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

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

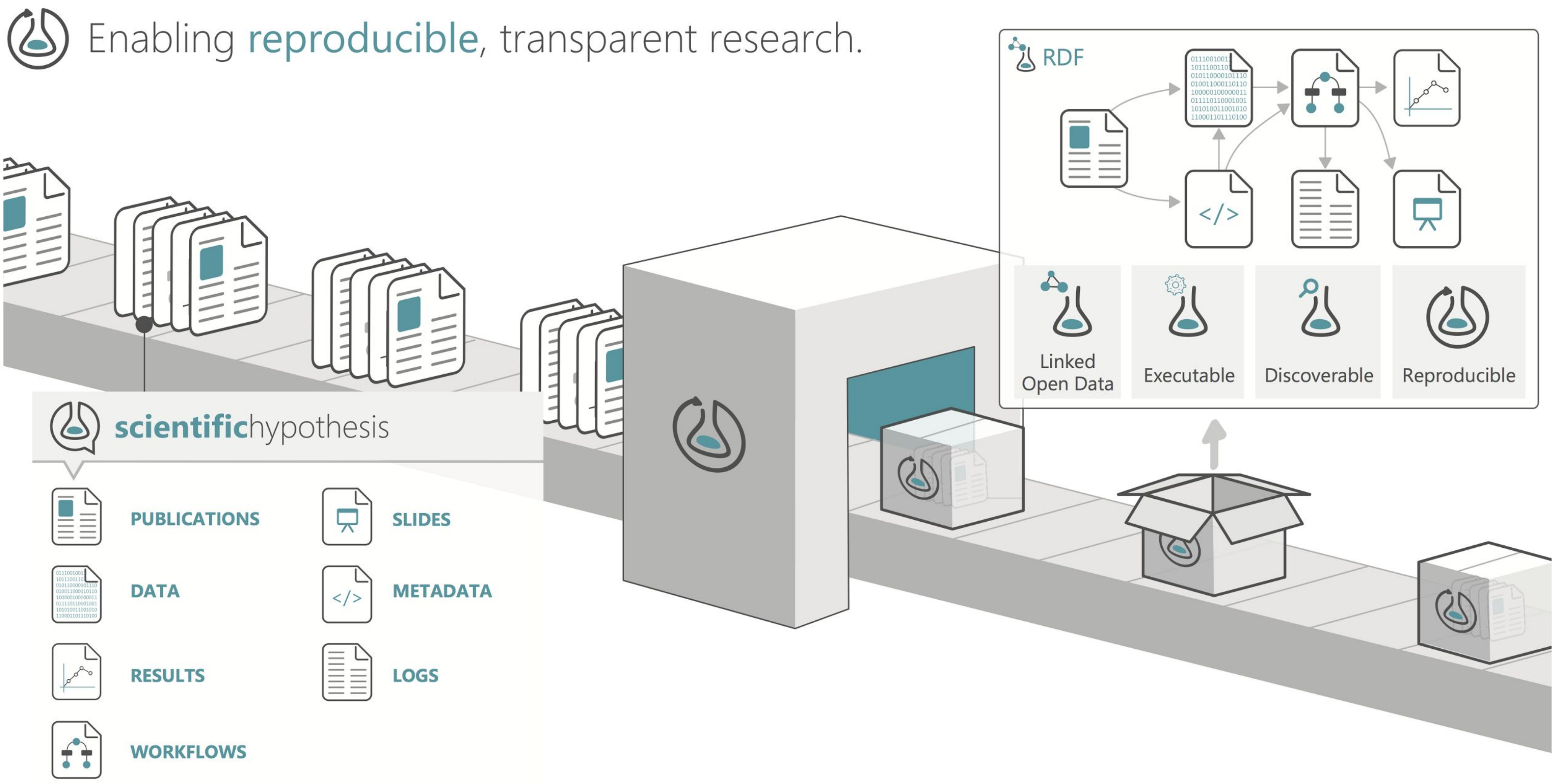
bcbio: Validated, scalable, community developed variant calling, RNA-seq and small RNA analysis (docs, BOSC 2016 talk: video, slides) (Brad Chapman et al.)

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

https://goo.gl/4peVam

ResearchObject.org standard overview



https://goo.gl/4peVam

CWL BACKENDS AS OF 2017/06/21

	Airflow	Arvados	Toil	Rabix Executor local & TES only	Ref. Impl. cwltool -- local only
amazon web services		✓	✓		
Microsoft Azure		✓	✓		
grid engine			✓		
Google Cloud Platform		✓	✓		
Software defined infrastructure IBM Spectrum LSF			✓		
Apache MESOS	✓		✓		
openstack			✓		
slurm		✓	✓		

Capabilities are self reported and CWL support can vary depending on configuration.

https://goo.gl/4peVam

CWL v1.0 released June 2016

http://www.commonwl.org/v1.0/

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Dan Leehr, Duke University
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