Searching for Cancer Biomarkers with Apache OODT

Rishi Verma
NASA Jet Propulsion Laboratory,
California Institute of Technology
February 27th, 2013

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NORTH AMERICA 2013
Open Source Community Leadership Drives
Enterprise-Grade Innovation

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Agenda

* Introduction
* Science of cancer biomarker research
* Apache OODT and data processing
* Example: EDRN LabCAS Proteomics Pipeline
* Tutorial: Build your own processing system

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Introduction

Rishi Verma

NASA Jet Propulsion Laboratory

- Software engineer specializing in data services for scientific discovery
- Involved in:
  - Cancer research
  - Mars Science Laboratory
  - Deep Space Network
  - CO2 data management
  - Earthquake data management
- Program management committee member and committer for Apache OODT

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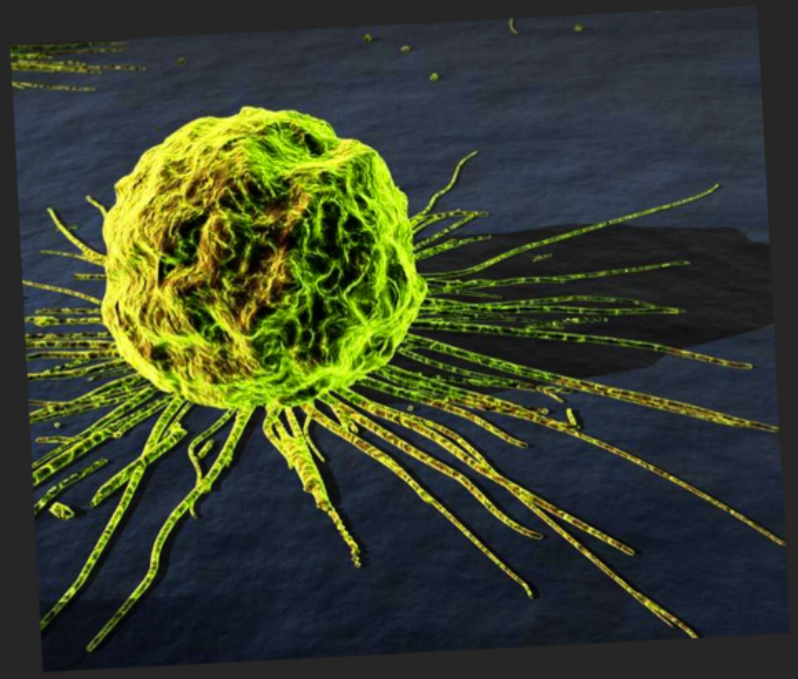
Science of cancer biomarker research



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Cancer biomarkers

- biological indicators
- used in many fields: medicine, biology, geology... etc.

"A biological molecule found in blood, other body fluids, or tissues that is a sign of a normal or abnormal process, or of a condition or disease."

- National Cancer Institute

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biomarkers

- biological indicators
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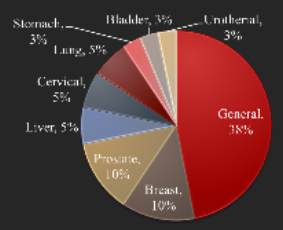
Cancer biomarkers: facts

Applications:

- Screening
- Early detection
- Treatment

Types

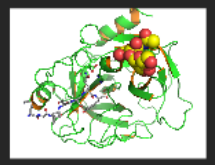
- Proteins
- Gene expression and DNA



Examples

Prostate specific antigen (PSA)

- Cancer type: prostate
- Substence type: glycoprotein
- Use: like other markers, currently screening is not recommended



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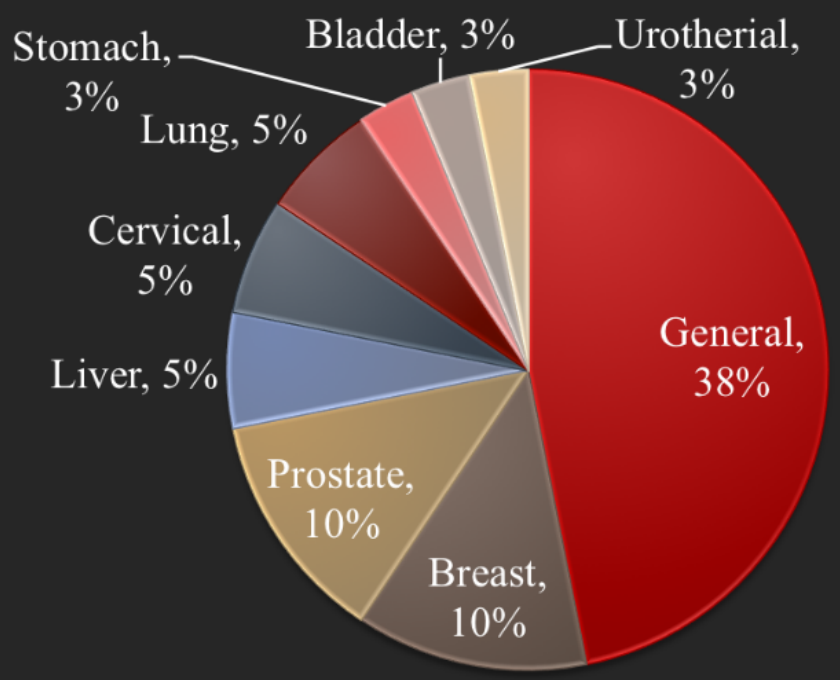

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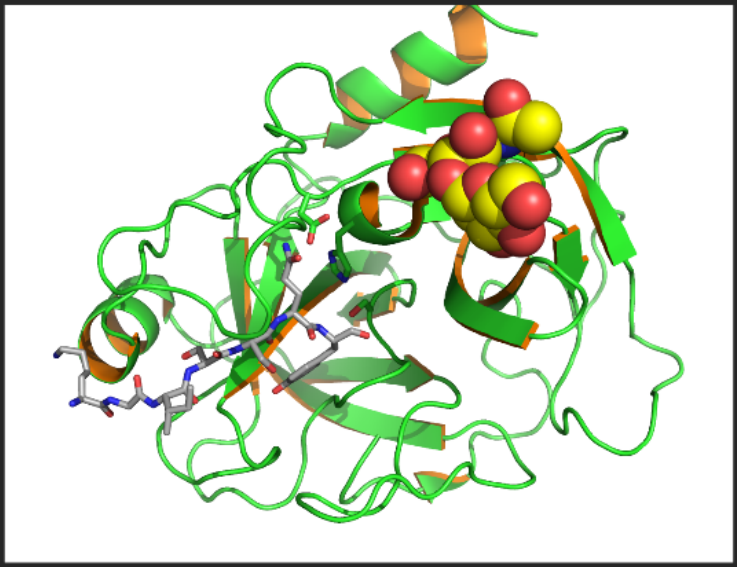

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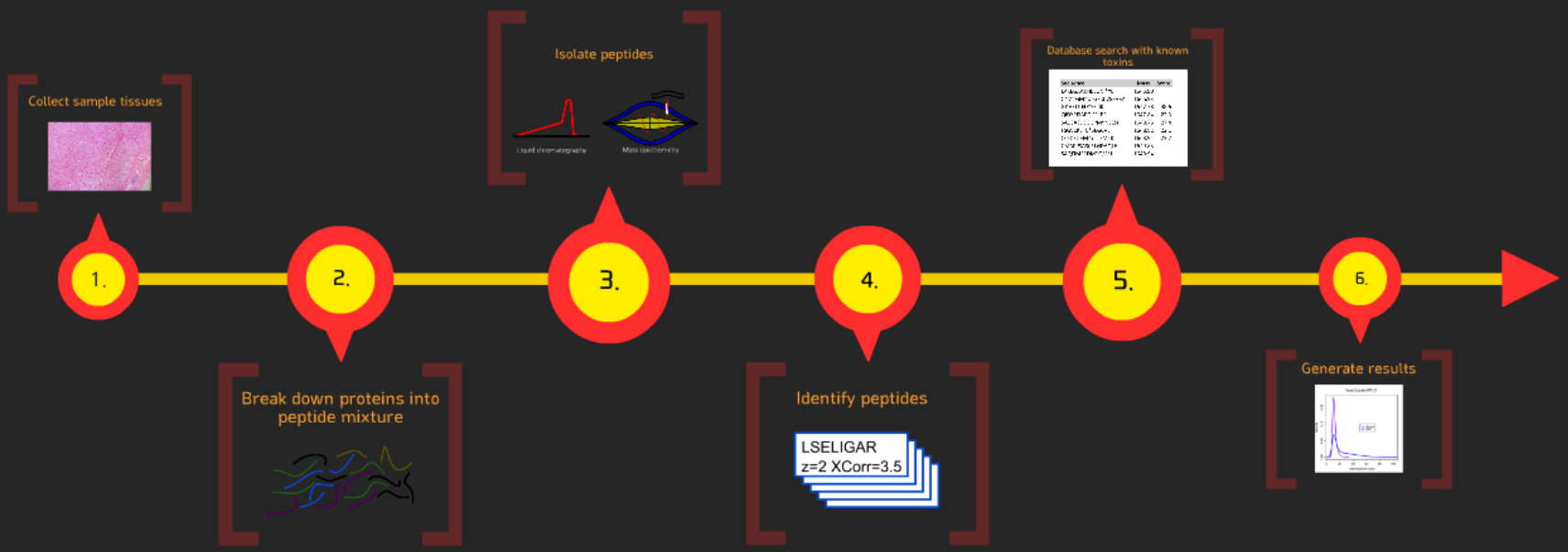
Cancer biomarker: discovery

Example: protein identification



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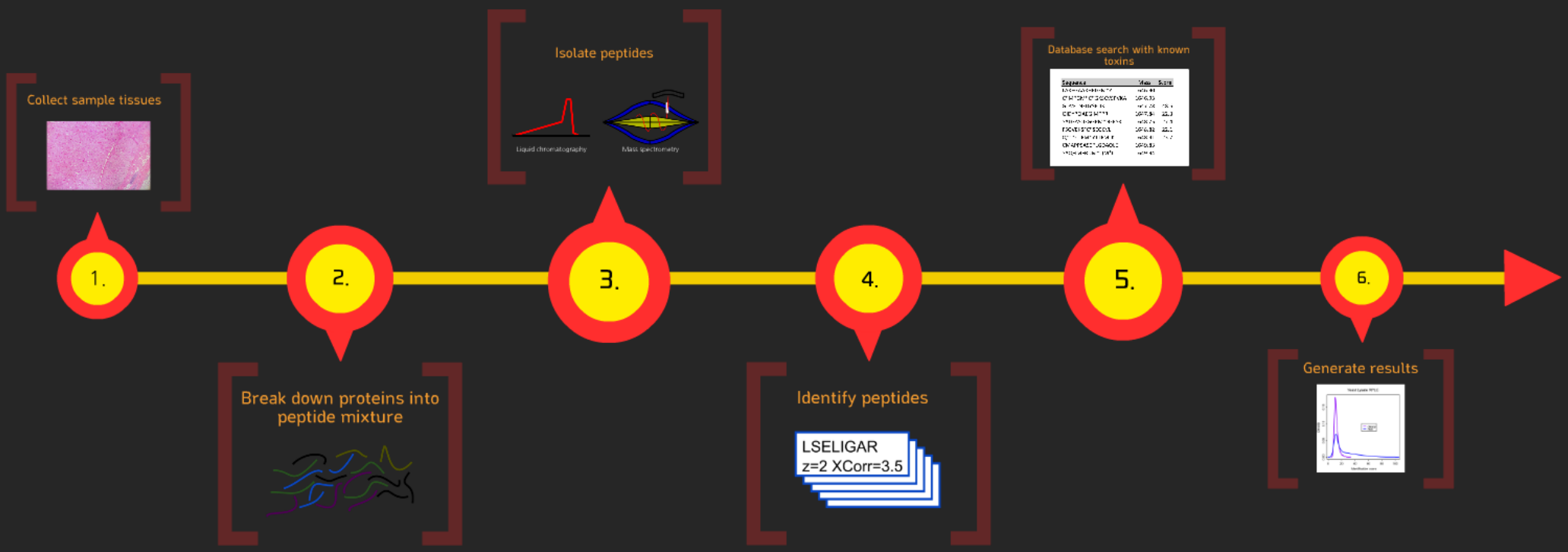
Cancer biomarker: discovery

Example: protein identification



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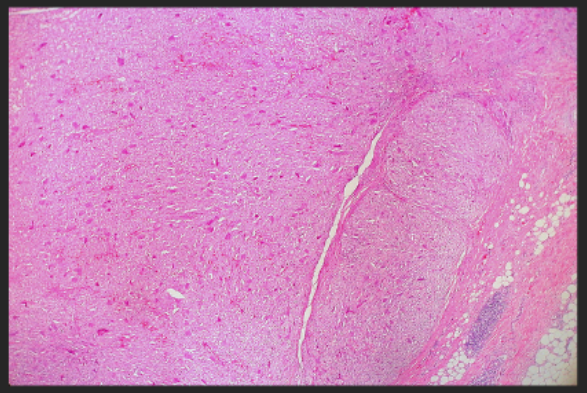
Collect sample tissues



1.

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2.

Break down proteins into peptide mixture

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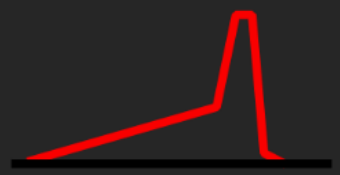
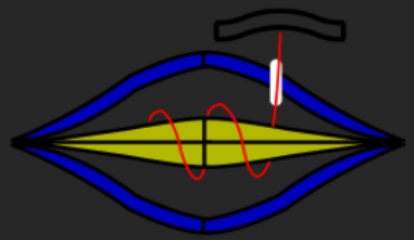
Isolate peptides



Liquid chromatography



Mass spectrometry

3.

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4.

Identify peptides

LSELIGAR
z=2 XCorr=3.5

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Database search with known toxins

Sequence	Mass	Score
LAKEGAAKHELGM*YL	1646.90	
C*M*GM*C*GKSCVSPVKA	1646.93	
GDVFTNFDYSELIK	1647.78	48.6
QIDYPEIAEGIM*PR	1647.84	22.3
SALGASLGGGPM*NEESR	1648.75	27.4
FSGVEKSFC*SEGCVL	1648.82	22.1
Q*C*CLEM*YTTEMLK	1648.91	23.7
CMAPPSASC*LGDAQLE	1649.83	
SAQFIMFRDM*QM*L	1649.94	

5.

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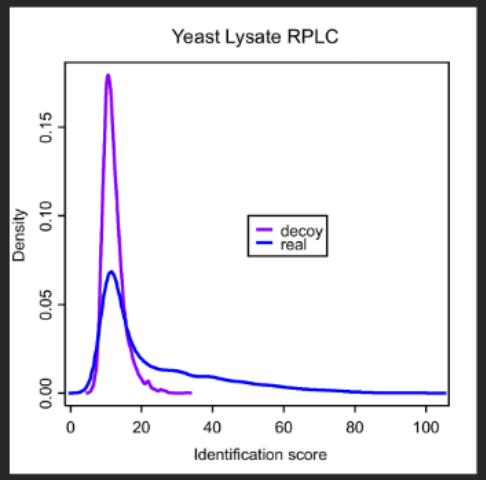
6.

Generate results



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Apache OODT and data processing

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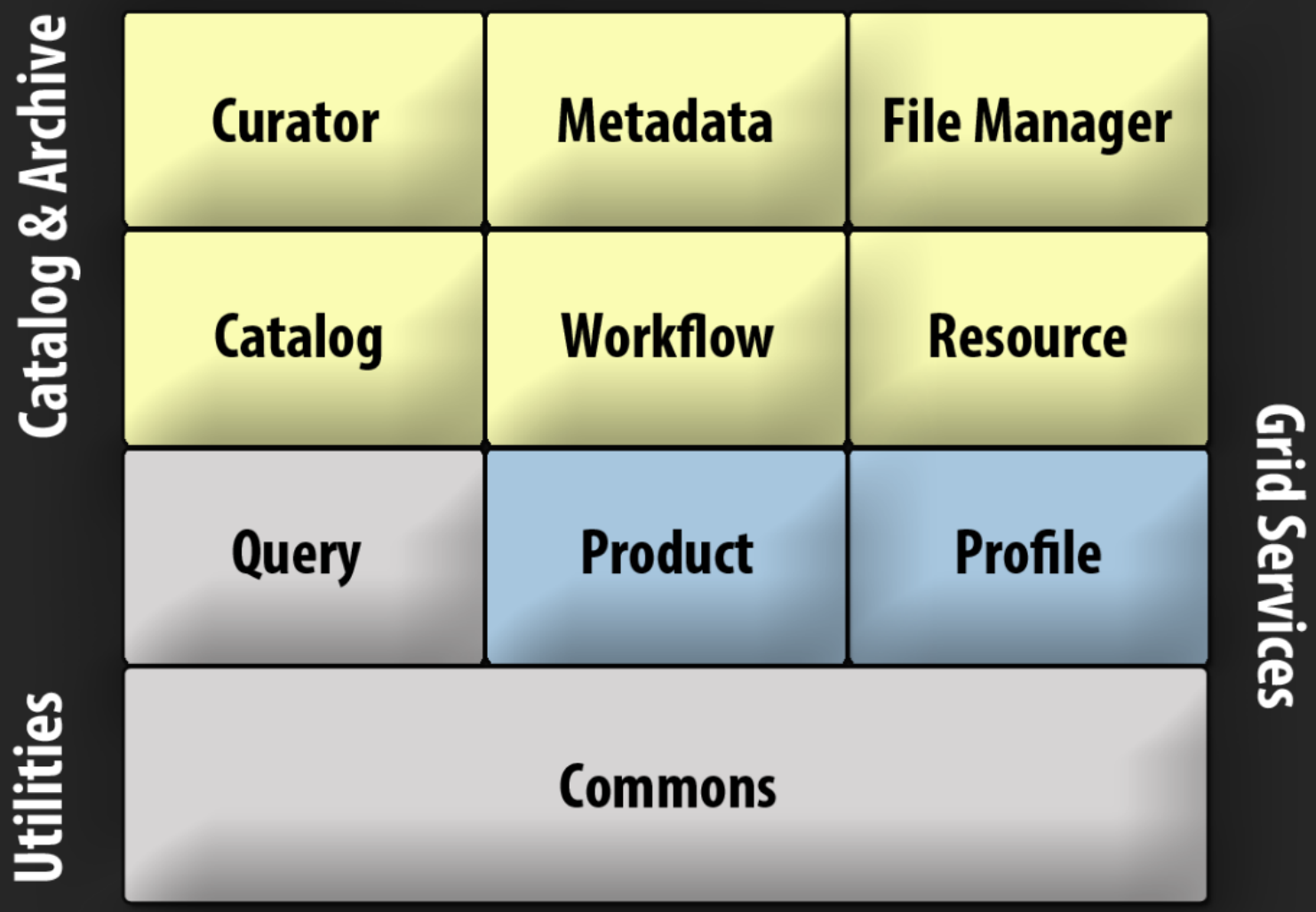
What is Apache OODT?



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What is Apache OODT

Catalog & Archive

Curator	Metadata	File Manager
Catalog	Workflow	Resource
Query	Product	Profile

Grid Services

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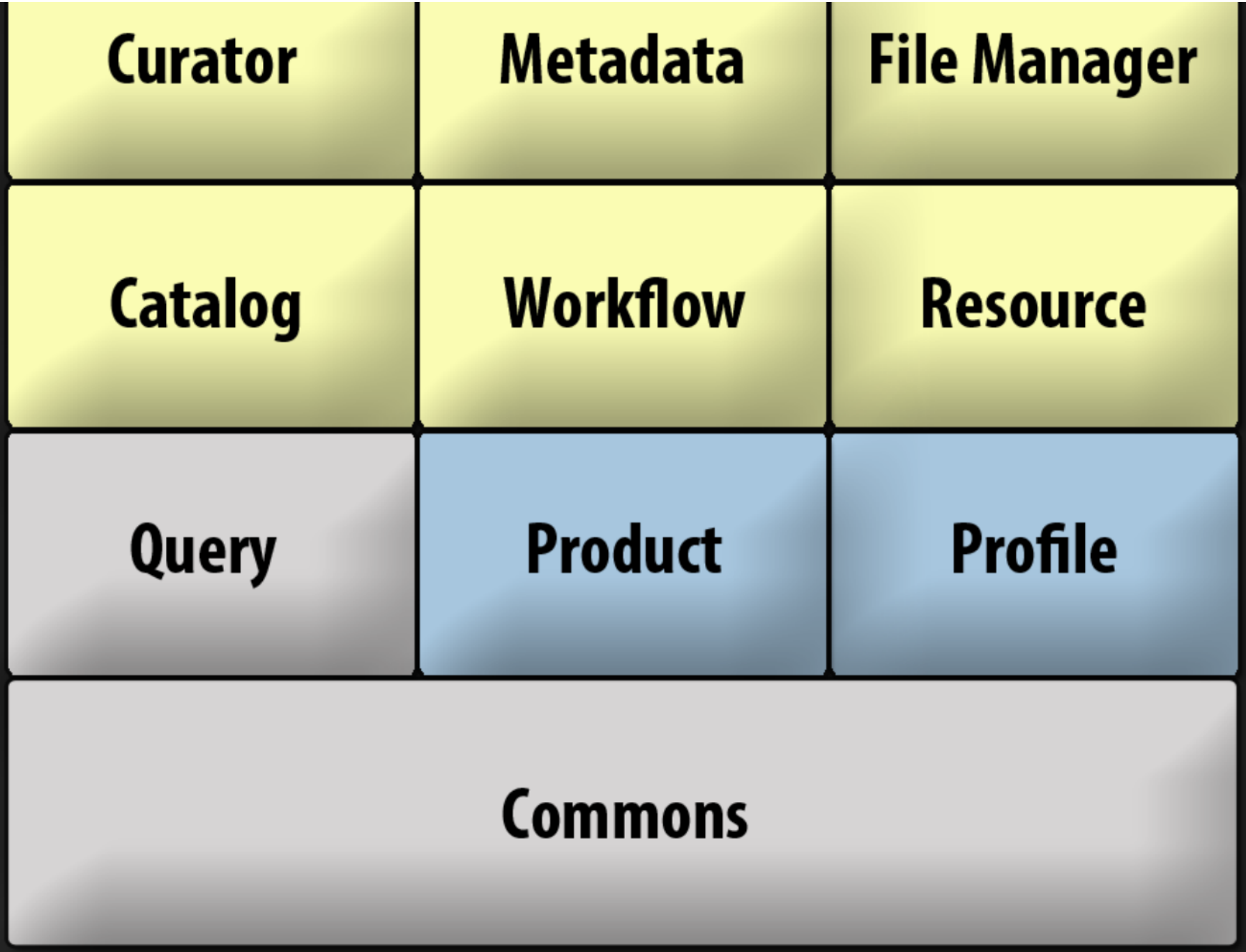

Grid Services

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Ca

Query

Product

Pr

Utilities

Commons

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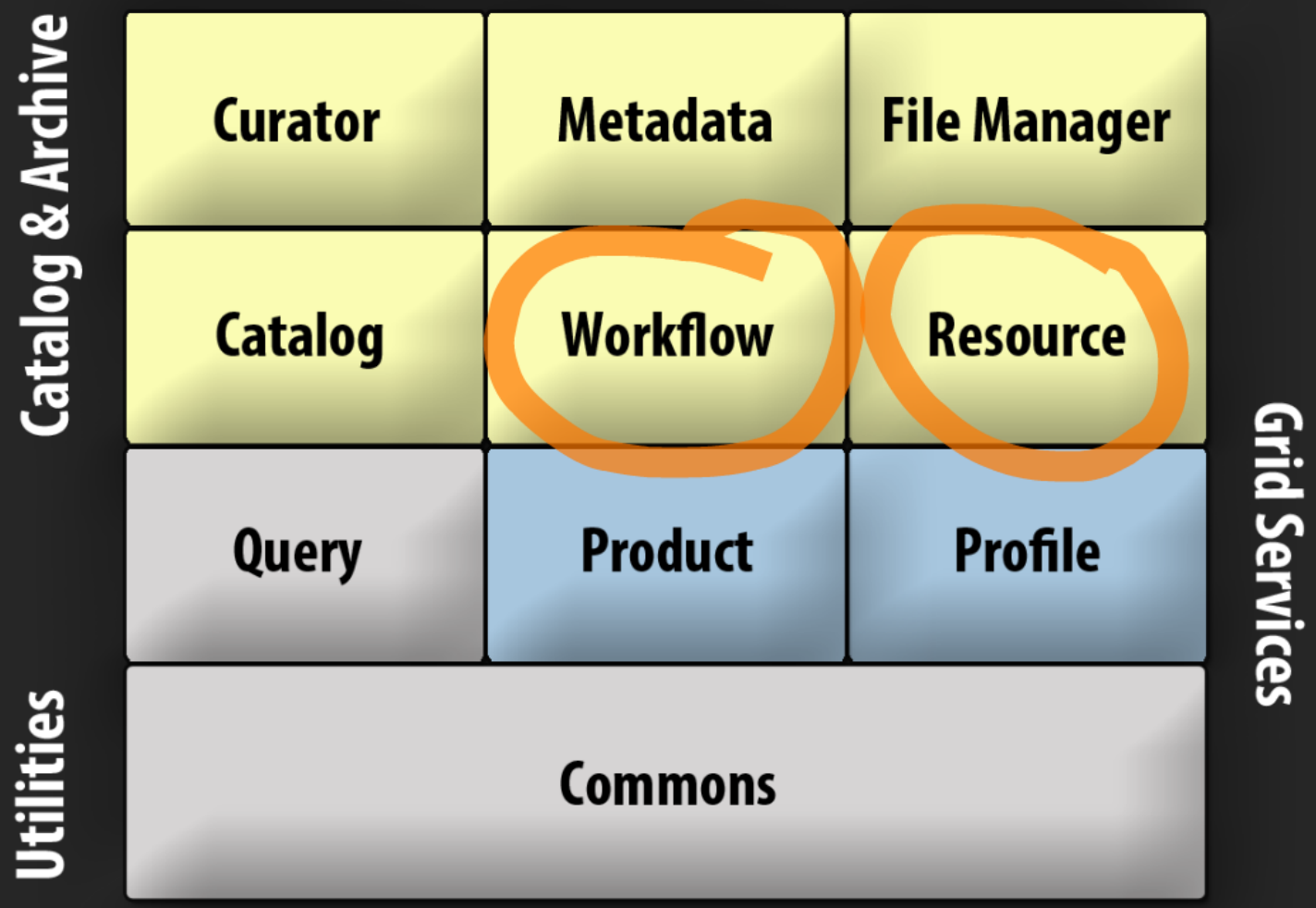
OODT Data Processing Components



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Process Control System (PCS)

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Archive Management

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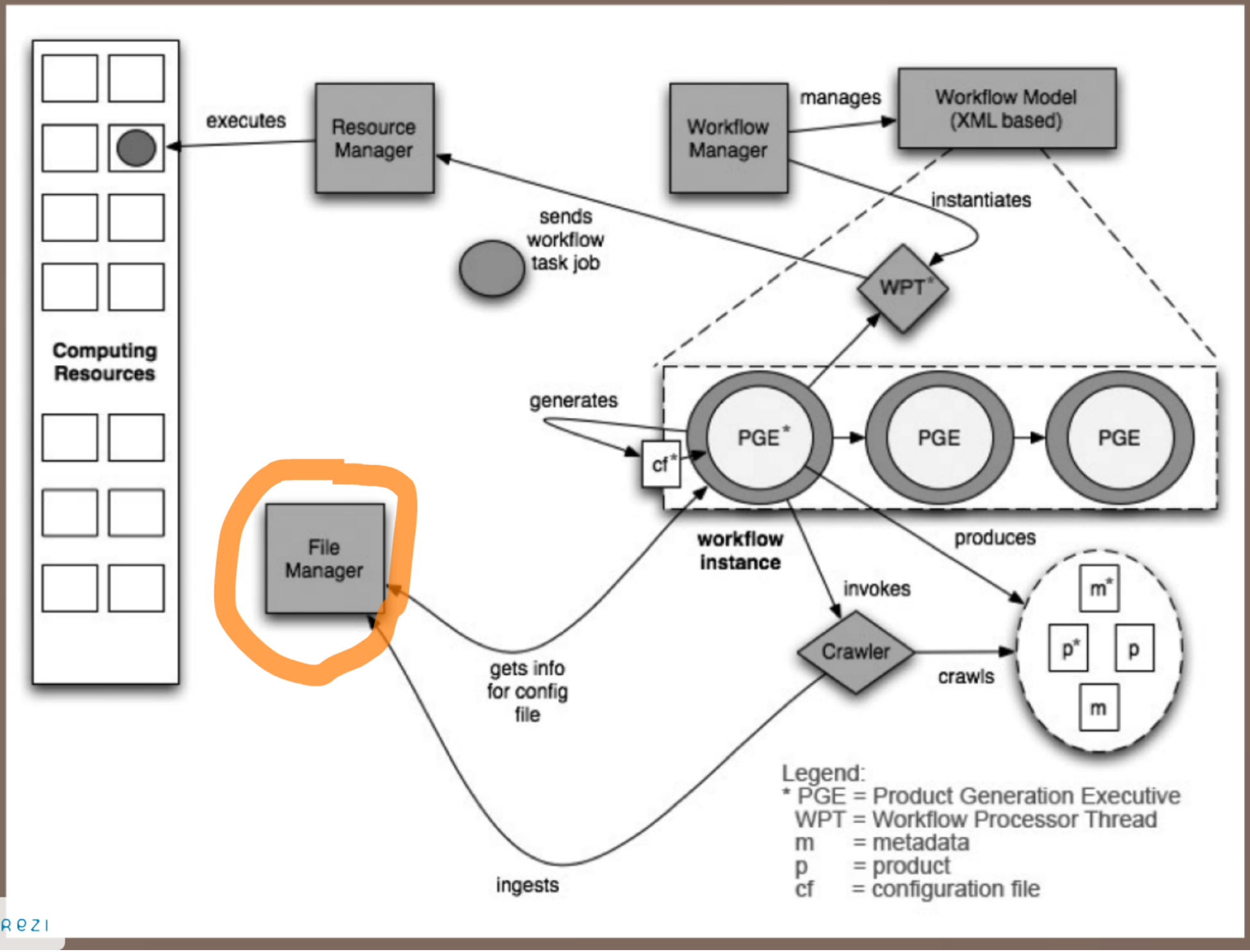
executes
Resource Manager
Workflow Manager
manages
Workflow Model (XML based)
instantiates
sends workflow task job
WPT*
Computing Resources
generates
cf*
PGE*
PGE
PGE
workflow instance
produces
File Manager
invokes
Crawler
crawls
m*
p*
p
m
gets info for config file
ingests
Legend:
* PGE = Product Generation Executive
WPT = Workflow Processor Thread
m = metadata
p = product
cf = configuration file

Process Control System (PCS)

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products

Workflow Manager

Compu

products

Science Algorithm Management

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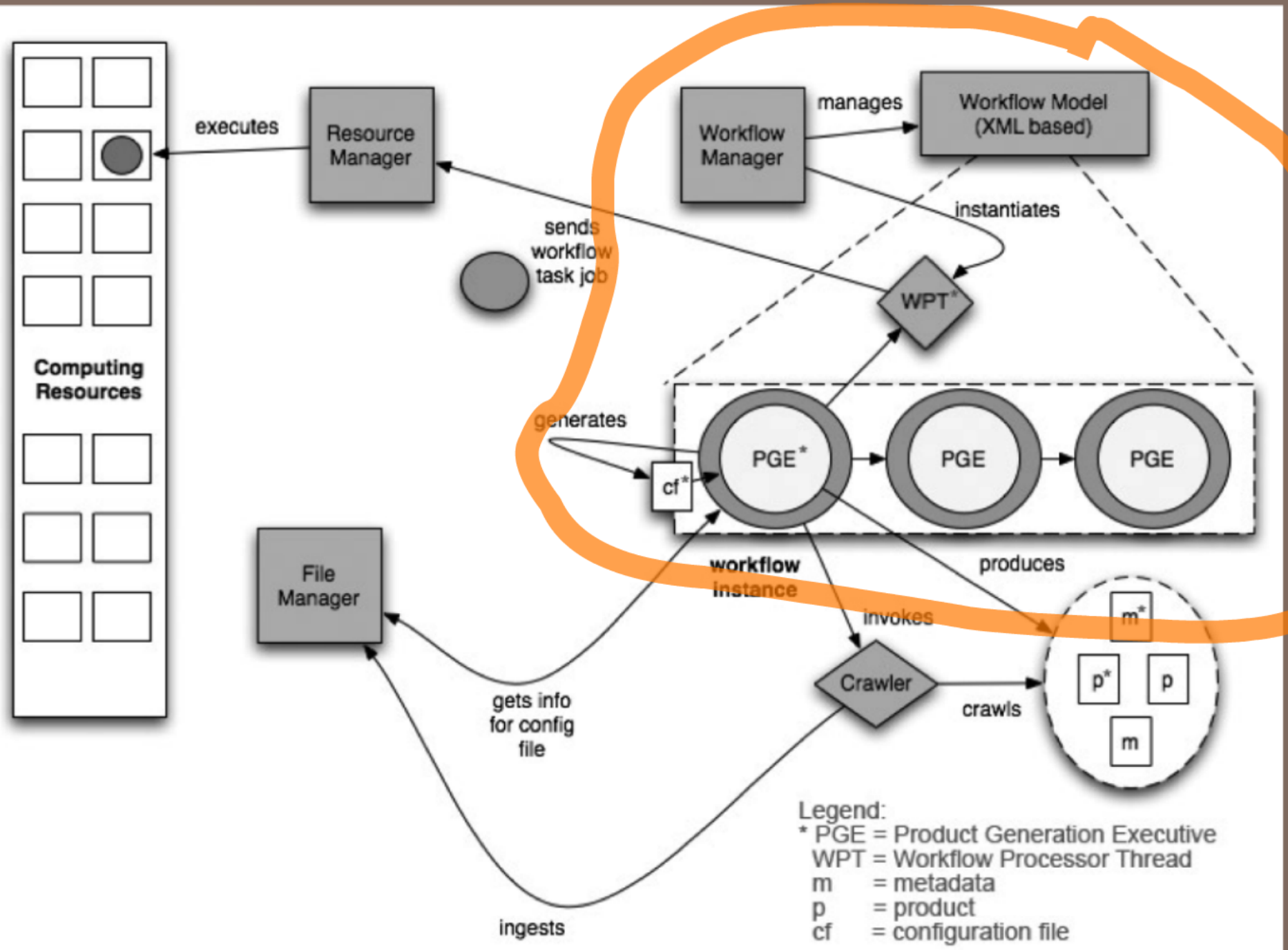
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Process Control System (PCS)

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Resource Manager

Computation Management

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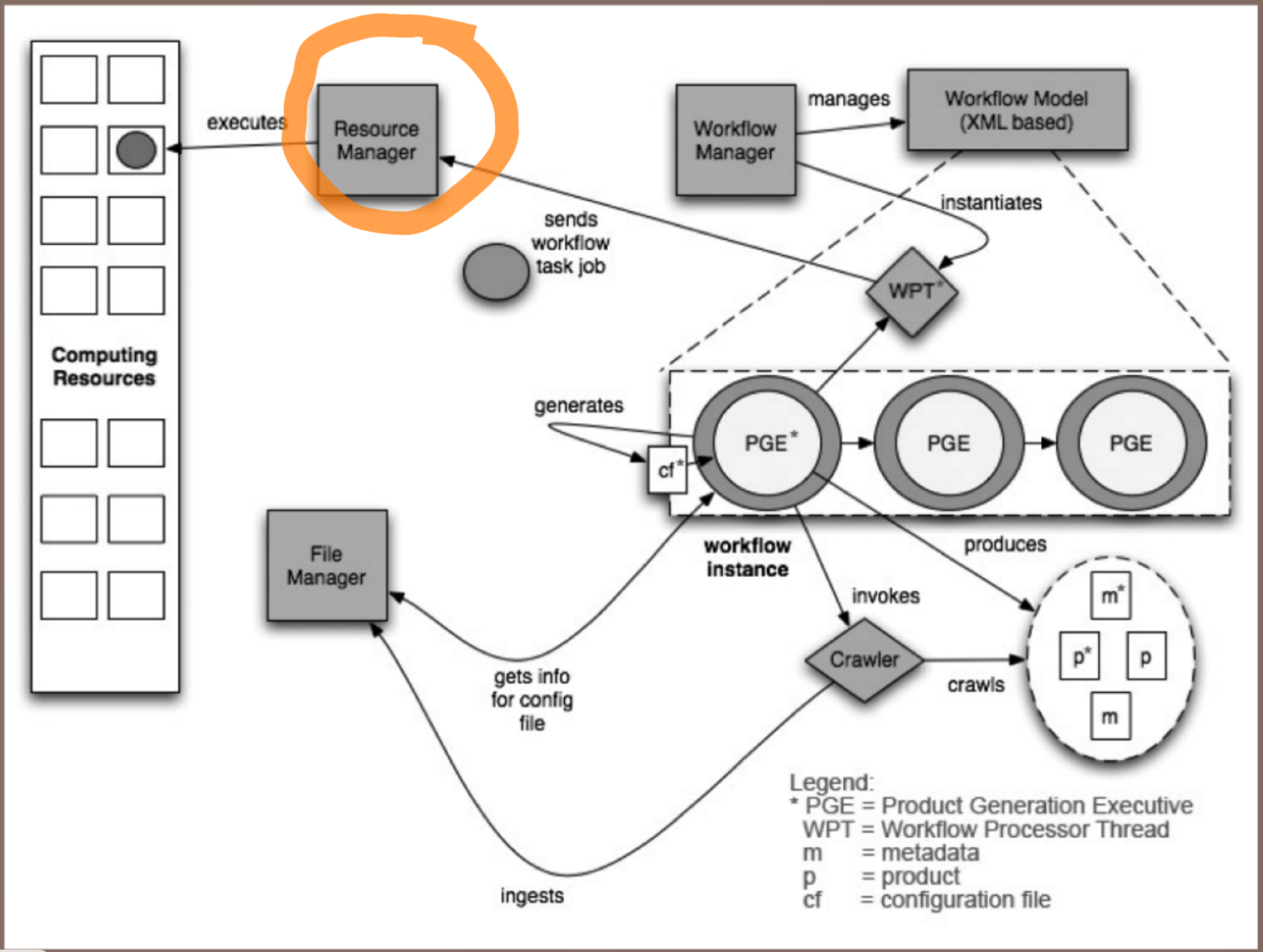
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Example: EDRN LabCAS Proteomics Pipeline

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National Cancer Institute

Early Detection Research Network

Biomarkers: the key to early detection

- Founded in 2000
- Objectives:
  - Identify clinically applicable cancer biomarkers
  - Connect disparately located researchers
  - Establish a national biomarker research infrastructure

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EDRN LabCAS and the Proteomics Pipeline

Laboratory Catalog and Archive Service (LabCAS)

- Data management infrsastructure for EDRN researchers
- Targeted at pre-publication, experimental research data

Proteomics Pipeline

- Centralized data processing system for LabCAS
- Configurable workflows for analyzing tissue sample data using diverse algorithms
- Generation of higher-level products

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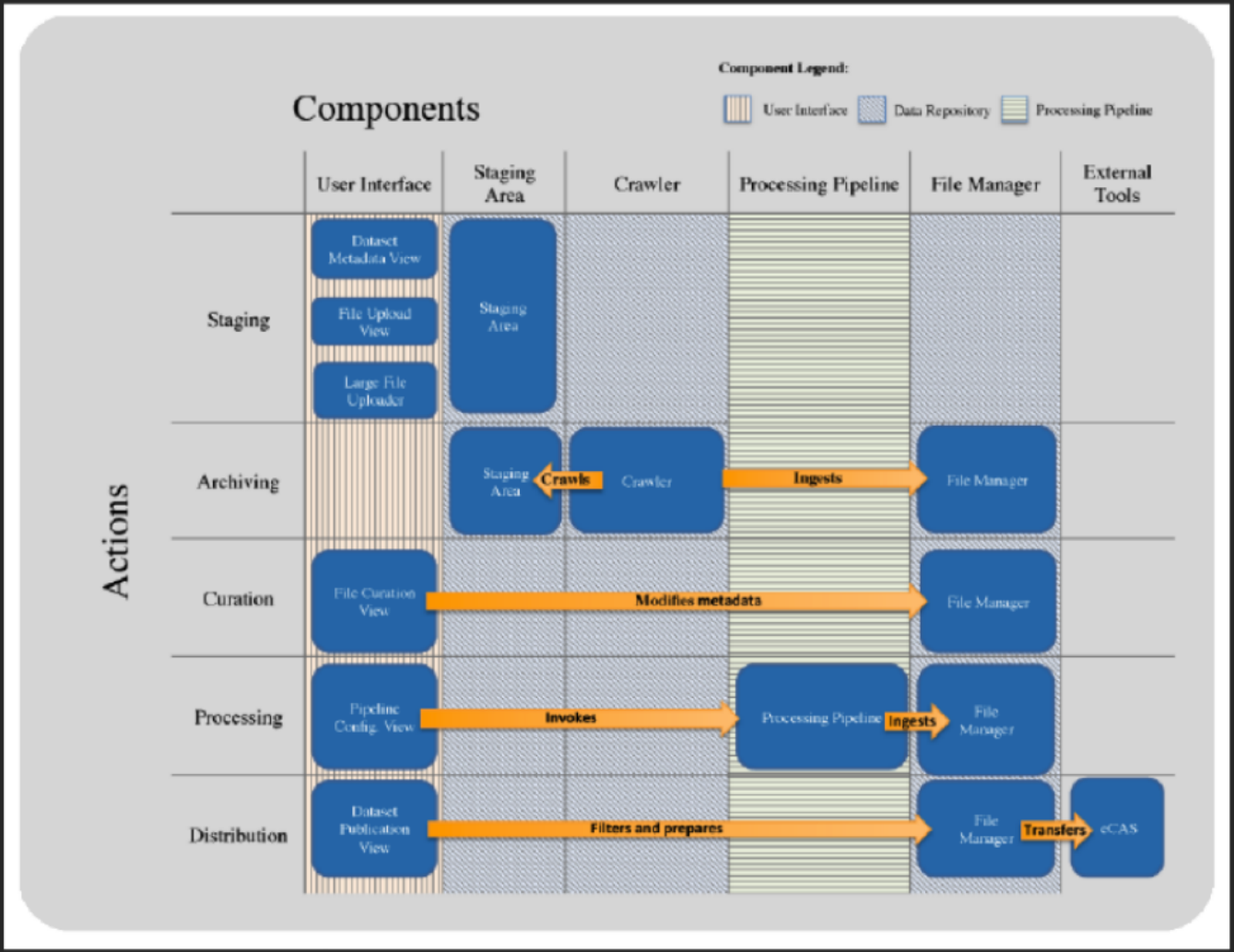
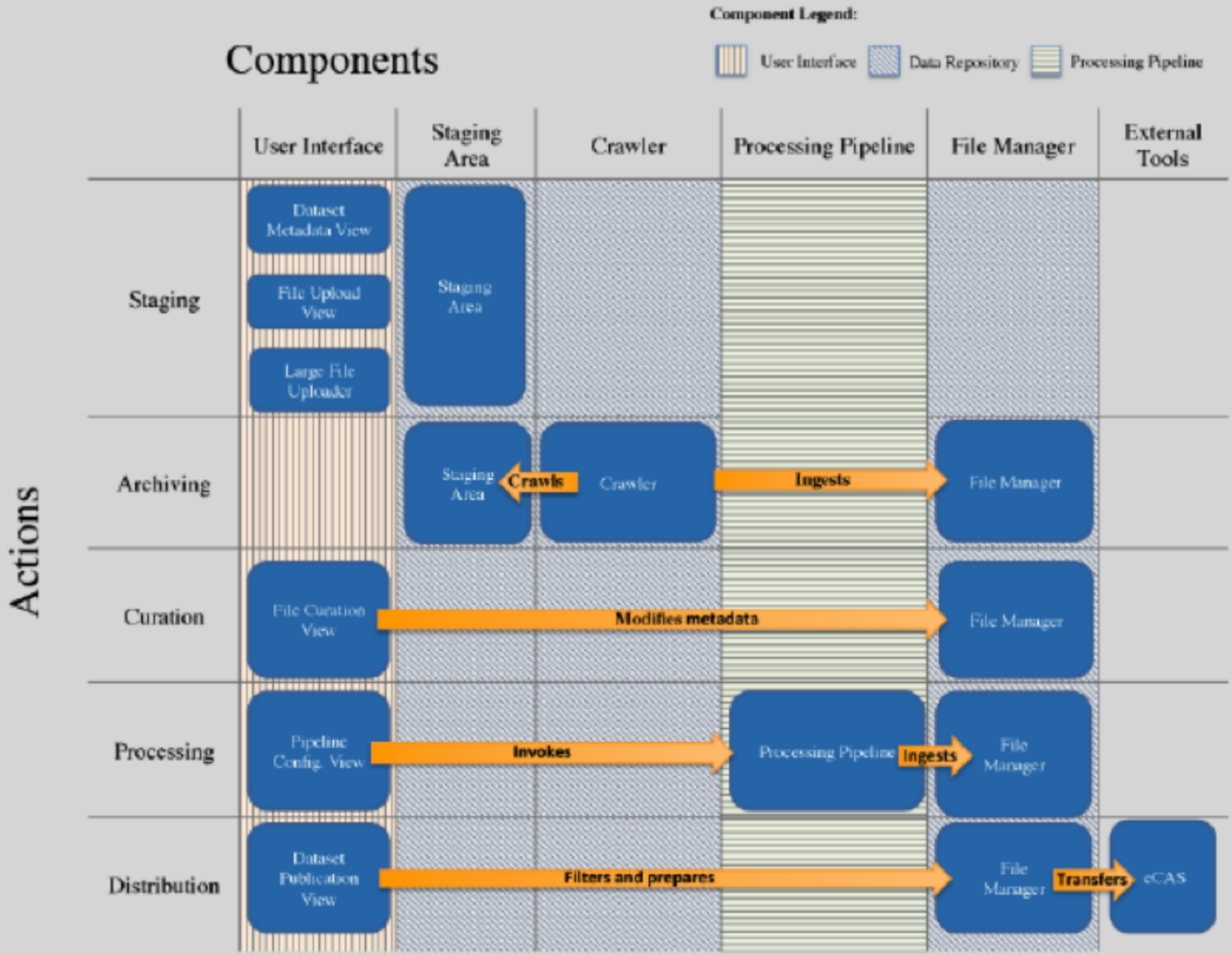
Leveraging the OODT framework




Component Legend:
User Interface
Data Repository
Processing Pipeline
Components
User Interface
Staging Area
Crawler
Processing Pipeline
File Manager
External Tools
Actions
Staging
Archiving
Curation
Processing
Distribution
Dataset Metadata View
File Upload View
Large File Uploader
Staging Area
Staging Area
Crawls
Crawler
Ingests
File Manager
File Curation View
Modifies metadata
File Manager
Pipeline Config. View
Invokes
Processing Pipeline
Ingests
File Manager
Dataset Publication View
Filters and prepares
File Manager
Transfers
eCAS

LabCAS Demonstration

http://goo.gl/24M4U

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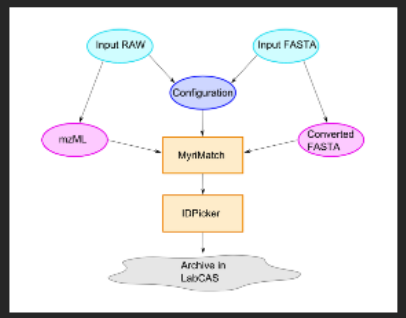
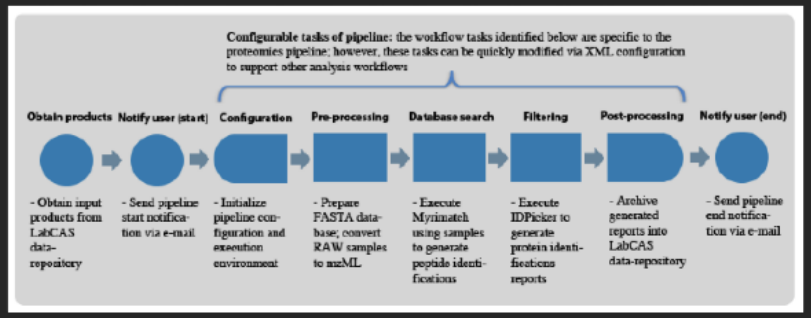
Proteomics Pipeline

- Centralize the the analysis of LabCAS data sets
- Make available a variety of analysis algorithms

Algorithm



Workflow Implementation



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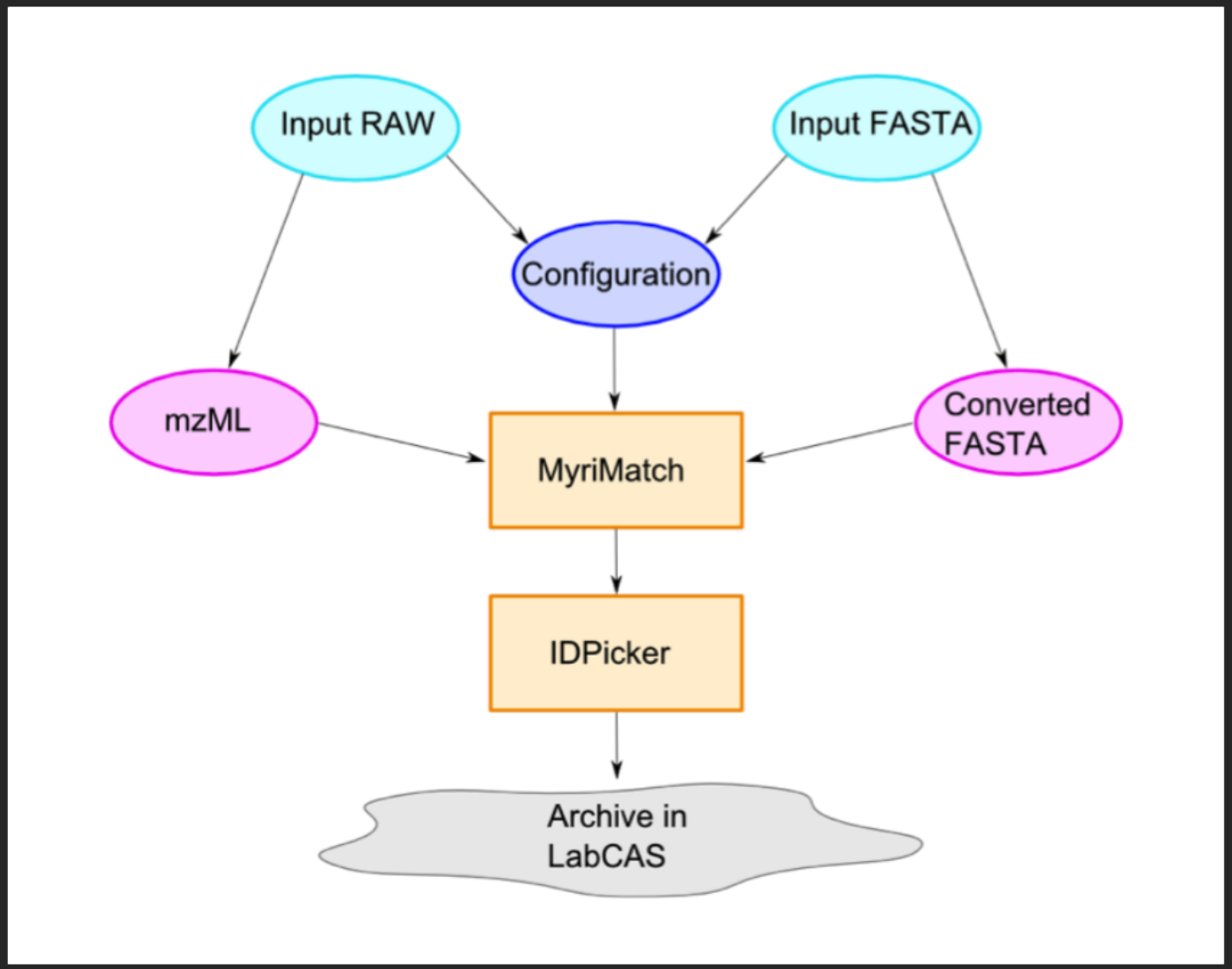
Algorithm



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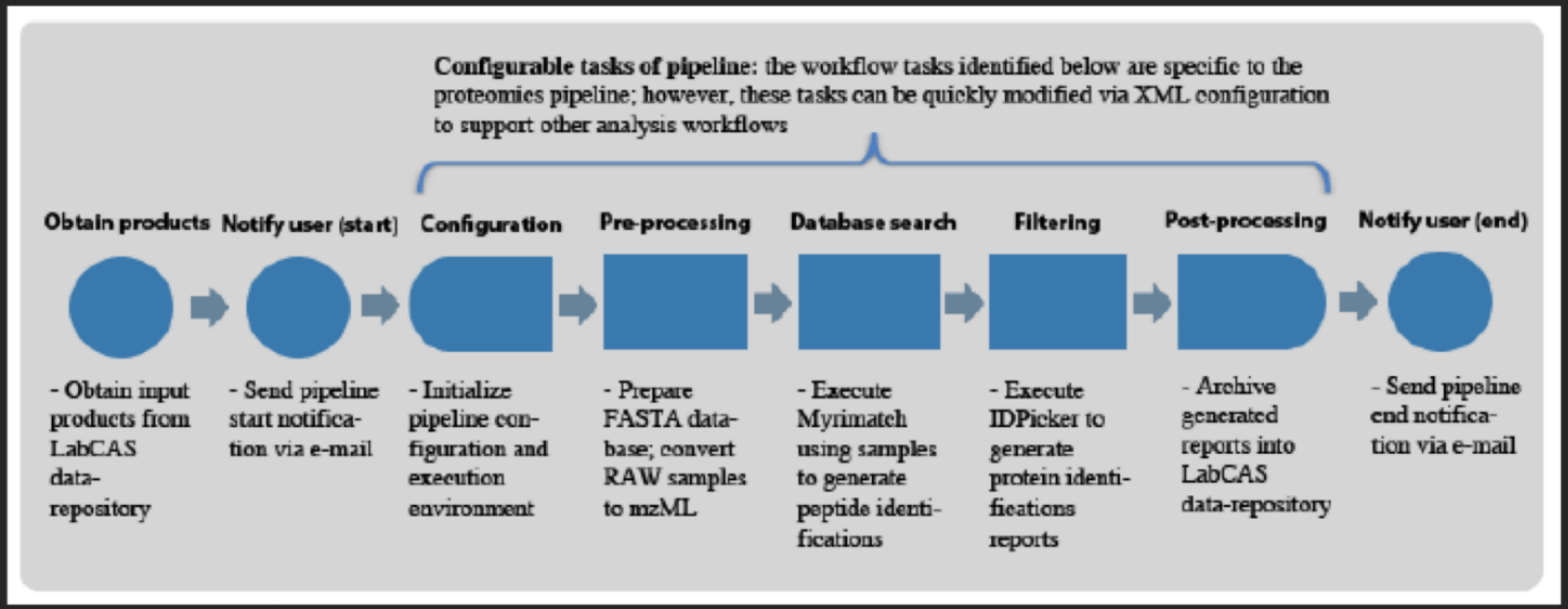

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Proteomics Pipeline Demonstration

http://goo.gl/7sZjl

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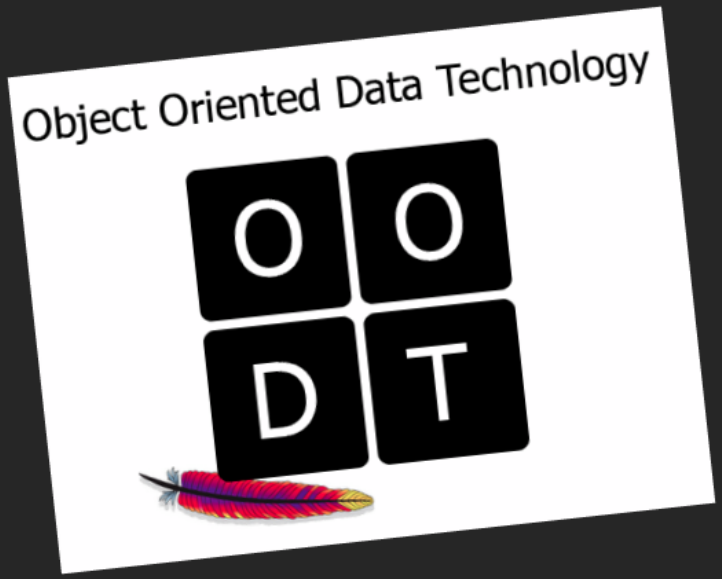
Tutorial: Build your own processing system



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Review of steps:

1. Download OODT PCS framework:
   - File Manager
   - Workflow Manager
   - Resource Manager
   - Crawler ...
2. Configure components
3. Wrap science algorithms using PGEs
4. Configure user interface

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Easier method?

Try Apache OODT's RADiX tool!

- Contains distribution of Apache OODT
- Convention over configuration
- Reduce ramp up time
- Eliminate some configuration

Details:

- Uses Apache Maven Archetype construct
- Auto-generation of OODT base project

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Using OODT RADiX

```
% mvn archetype:generate -DarchetypeGroupId=org.apache.oodt -DarchetypeArtifactId=radix-archetype -DarchetypeVersion=0.6-SNAPSHOT -Doodt=0.6-SNAPSHOT -DgroupId=com.mycompany -DartifactId=dms -Dversion=0.1-SNAPSHOT
% cd dms; mvn package
% tar -xvf distribution/target/dms-distribution-0.1-SNAPSHOT-bin.tar.gz -C ../oodt-deploy
% cd ../oodt-deploy
% ./bin/oodt start
```

Try out the base deployment, then:

- Customize your workflows by wrapping science algorithms
- Customize your resource management strategy
- Customize your archival strategy

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Using OODT RADiX

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deploy
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Thanks! Questions?

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- Cameron Goodale, NASA Jet Propulsion Laboratory
- David Tabb, Vanderbilt University Medical Center
- Chris Mattmann, NASA Jet Propulsion Laboratory
- Paul Ramirez, NASA Jet Propulsion Laboratory

Bibliography:
- http://www.cancer.gov/cancertopics/factsheet/Detection/tumor-markers
- http://en.wikipedia.org/wiki/Cancer_biomarkers
- http://sunset.usc.edu/~mattmann/pubs/SMCIT09.pdf

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