Manifest Specification draft for FAIR Containerized Computational Software (FAIR-CCS)

Mylene Simon

Software Engineer & WIPP Lead Developer

Prometheus Computing LLC

National Institute of Standards and Technology (NIST)

2nd International Workshop on FAIR Containerized Computational Software - December 5, 2023

Presentation outline

- Context: the Web Image Processing Pipelines (WIPP) project and plugin manifest

- FAIR-CCS manifest
    - General overview
    - Metadata/General information section
    - Inputs and outputs section
    - User Interface (UI) section
    - Resource requirements section

Lowering barriers for accessing, processing and exploring large-scale digital image collections - Key challenges

Big Data Management

- Data sharing and dissemination
  - In the past, hard drives exchanges between users and teams, desktop solutions
  - Need for scalable and interactive visualizations
- Computational scalability
  - Memory-consuming complex algorithms applied to Tera-Byte-sized datasets
  - Limitation of desktop machines, Use of cluster or cloud resources for advanced users

Heterogeneity in Image Processing software and algorithms

- Algorithms come from many libraries and programming languages
- Hardware and OS requirements for installation and execution
- Learning curve for end-user
- How to chain algorithms into complex workflows?

Traceability of data and software-based measurements

- How to link a value to specific dataset, software, algorithm, formula, parameters?
- Managing versions of software/algorithm

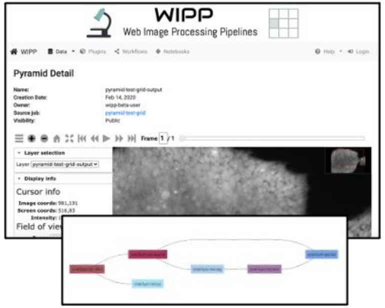
FAIR software, DevOps and productivity

- How to make computational tools/software Findable, Accessible, Interoperable and Reusable?
- How to decouple computational tools from execution platforms and facilitate their development, maintenance, integration and deployment?

Current solutions using FAIR-CCS at NIST: WIPP Platform, Plugins, and Plugin Registry

WIPP Platform

Open-source web-based algorithmic plugin platform for distributed computations, online data exploration and trusted image-based measurements from terabyte-sized images



Pyramid Detail

Name: pyramid-test-grid-output
Creation Date: Feb 14, 2020
Owner: wipp-beta-user
Source job: pyramid-test-grid
Visibility: Public

Frame 1 / 1

Layer selection

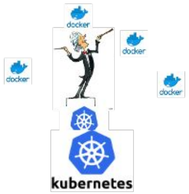
Layer pyramid-test-grid-output

Display info

Cursor info

Image coords: 981,191
Screen coords: 516,83
Intensity:

Field of vie

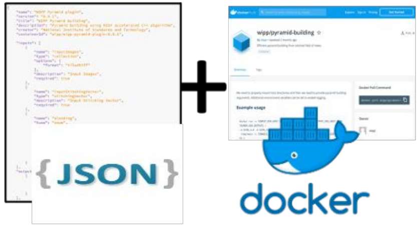


Cluster and cloud-ready

Source code plus deployment instructions:
https://github.com/usnistgov/WIPP

WIPP Plugins

Interoperable containerized algorithmic plugins associated with a JSON plugin manifest .

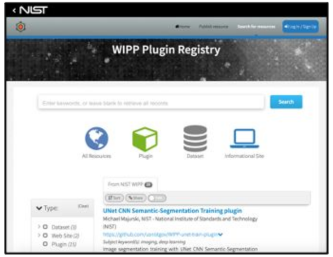


Compatible with Docker, Singularity, Kubernetes, Slurm and Common Workflow Language (CWL).

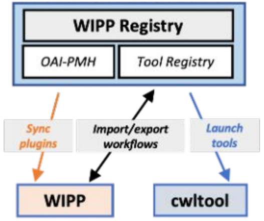
Template:
https://github.com/usnistgov/fair-chain-compute-container

WIPP Plugin Registry

Registry for storing, sharing and searching interoperable containerized plugins and computational workflows



UNet CNN Semantic-Segmentation Training plugin
Michael Majurski, NIST - National Institute of Standards and Technology (NIST)
https://github.com/usnistgov/WIPP-unet-train-plugin
Subject keyword(s): imaging, deep learning
Image segmentation training with UNet CNN Semantic-Segmentation



Source code and deployment instructions:
https://github.com/usnistgov/WIPP-Registry

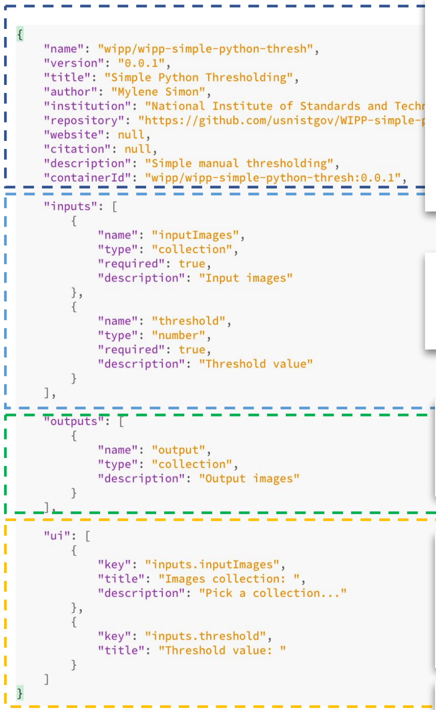
The WIPP Registry is powered by the NIST Configurable Data Curation System (CDCS)

https://cdcs.nist.gov/

FAIR-CCS manifest draft

FAIR-CCS manifest: manifest describing inputs, outputs, requirements, UI and general information about a containerized computational software

- Documentation and links to examples:
  - https://github.com/usnistgov/fair-chain-compute-container
- Online plugin manifest generation and validation tool:
  - https://usnistgov.github.io/WIPP-Plugin-Manifest-generator/
- FAIR-CCS Manifest JSON schema
  - Draft JSON schema available at https://github.com/usnistgov/fair-chain-compute-container/blob/master/schema/manifest.schema.json



```
{
    "name": "wipp/wipp-simple-python-thresh",
    "version": "0.0.1",
    "title": "Simple Python Thresholding",
    "author": "Mylene Simon",
    "institution": "National Institute of Standards and Techr
    "repository": "https://github.com/usnistgov/WIPP-simple-p
    "website": null,
    "citation": null,
    "description": "Simple manual thresholding",
    "containerId": "wipp/wipp-simple-python-thresh:0.0.1",
    "inputs": [
        {
            "name": "inputImages",
            "type": "collection",
            "required": true,
            "description": "Input images"
        },
        {
            "name": "threshold",
            "type": "number",
            "required": true,
            "description": "Threshold value"
        }
    ],
    "outputs": [
        {
            "name": "output",
            "type": "collection",
            "description": "Output images"
        }
    ],
    "ui": [
        {
            "key": "inputs.inputImages",
            "title": "Images collection: ",
            "description": "Pick a collection..."
        },
        {
            "key": "inputs.threshold",
            "title": "Threshold value: "
        }
    ]
}
```

Information about the software:
- name, version, description
- Docker image to use

Inputs description
- name, type, description

Outputs description
- name, type, description

UI description
- additional information to display on the form

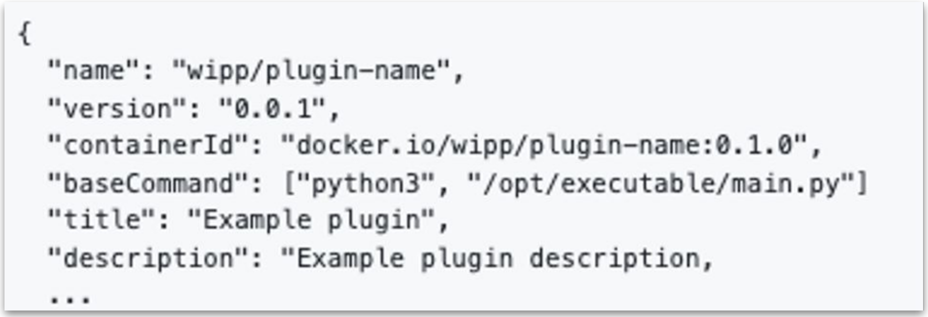
Resource requirements
- optional resource/hardware requirements

FAIR-CCS manifest (JSON file)

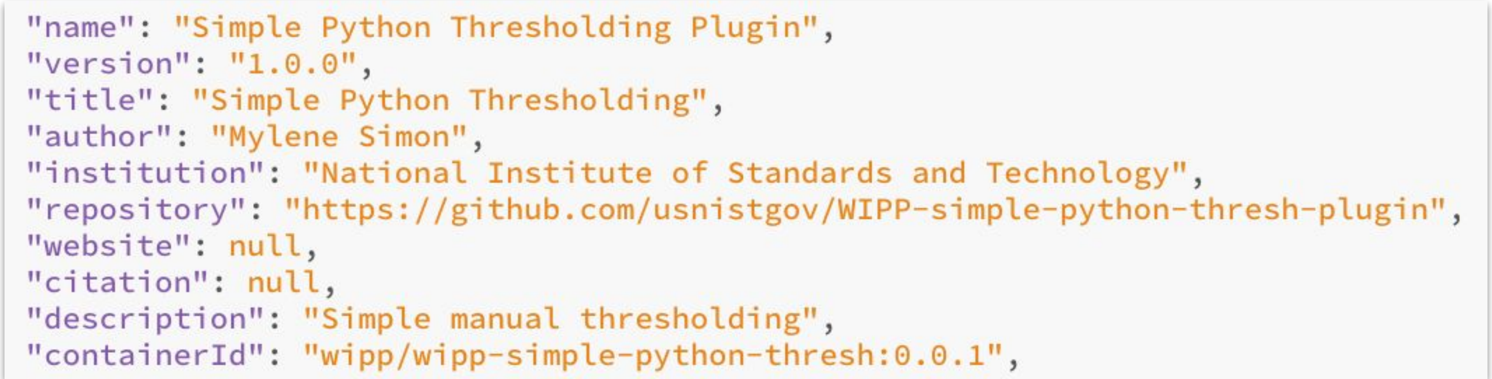
FAIR-CCS manifest: general information

General information about the containerized software

- Required: name, version, title, description, containerId
- Optional: institution, repository, website, citation, baseCommand



```
{
  "name": "wipp/plugin-name",
  "version": "0.0.1",
  "containerId": "docker.io/wipp/plugin-name:0.1.0",
  "baseCommand": ["python3", "/opt/executable/main.py"]
  "title": "Example plugin",
  "description": "Example plugin description,
  ...
```



```
"name": "Simple Python Thresholding Plugin",
"version": "1.0.0",
"title": "Simple Python Thresholding",
"author": "Mylene Simon",
"institution": "National Institute of Standards and Technology",
"repository": "https://github.com/usnistgov/WIPP-simple-python-thresh-plugin",
"website": null,
"citation": null,
"description": "Simple manual thresholding",
"containerId": "wipp/wipp-simple-python-thresh:0.0.1",
```

FAIR-CCS manifest: inputs section

Description of inputs

Required properties:

“name”, “type”, “description”

Optional properties:

“required”, “options”

Supported data types:

"collection” (collection of Images),

"stitchingVector” (MIST format),

"pyramid” (DeepZoom format),

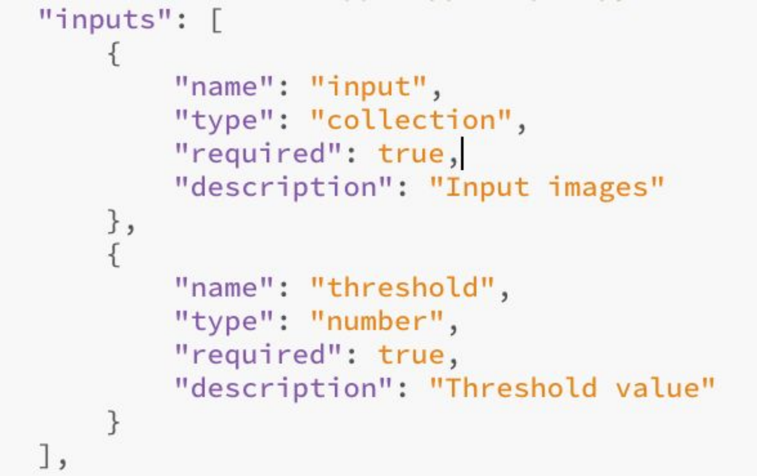
"tensorflowModel” (AI model),

"csvCollection” (collection of CSV files),

“genericData” (other data),

"notebook” (Jupyter notebook),

"string", "number", "integer", "enum", "array", "boolean"



```
"inputs": [
    {
        "name": "input",
        "type": "collection",
        "required": true,
        "description": "Input images"
    },
    {
        "name": "threshold",
        "type": "number",
        "required": true,
        "description": "Threshold value"
    }
],
```

FAIR-CCS manifest: outputs section

Description of outputs

Required properties:

“name”, “type”, “description”

Supported data types:

"collection” (collection of Images),

"stitchingVector” (MIST format),

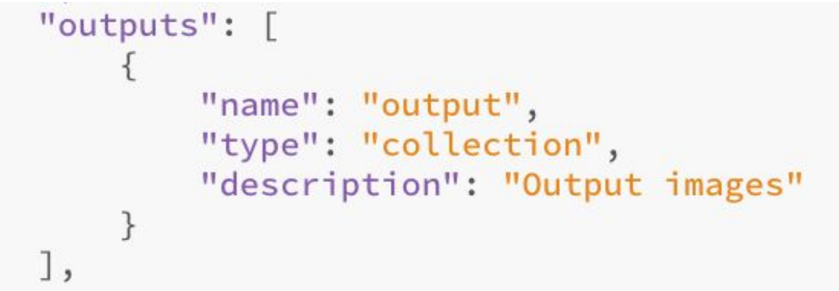
"pyramid” (DeepZoomWeb format),

"tensorflowModel” (AI model),

“tensorboardLogs” (logs for Tensorboard visualization),

"csvCollection” (collection of CSV images),

“genericData” (other data)

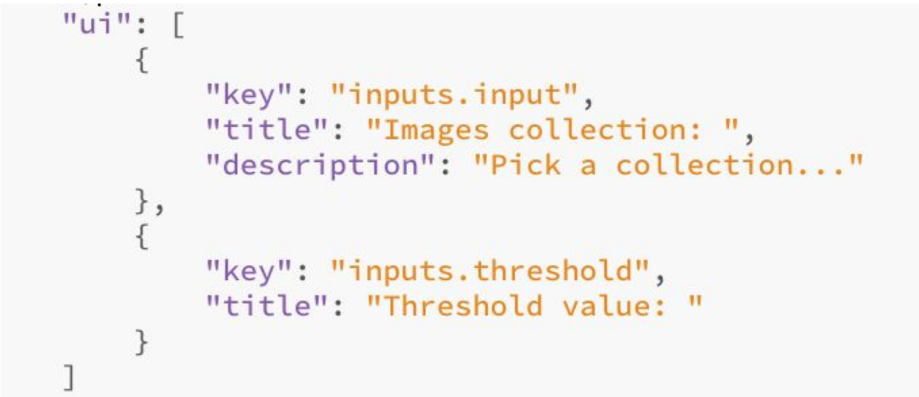


```
"outputs": [
    {
        "name": "output",
        "type": "collection",
        "description": "Output images"
    }
],
```

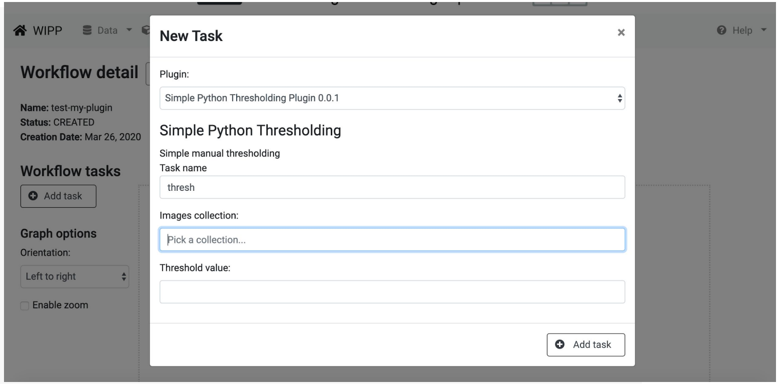
FAIR-CCS manifest: UI section

Description of UI

- One UI description per input
  - “key”: inputs.inputName (required)
  - “title”: input field label in form (required)
  - “description”: placeholder for string input field (optional)
- Advanced options not shown here (conditional visibility, binds between fields, etc.)



```
"ui": [
    {
        "key": "inputs.input",
        "title": "Images collection: ",
        "description": "Pick a collection..."
    },
    {
        "key": "inputs.threshold",
        "title": "Threshold value: "
    }
]
```



Name: test-my-plugin
Status: CREATED
Creation Date: Mar 26, 2020

Orientation: Left to right

New Task ×

Plugin: Simple Python Thresholding Plugin 0.0.1

Simple Python Thresholding

Simple manual thresholding

Task name: thresh

Images collection: Pick a collection...

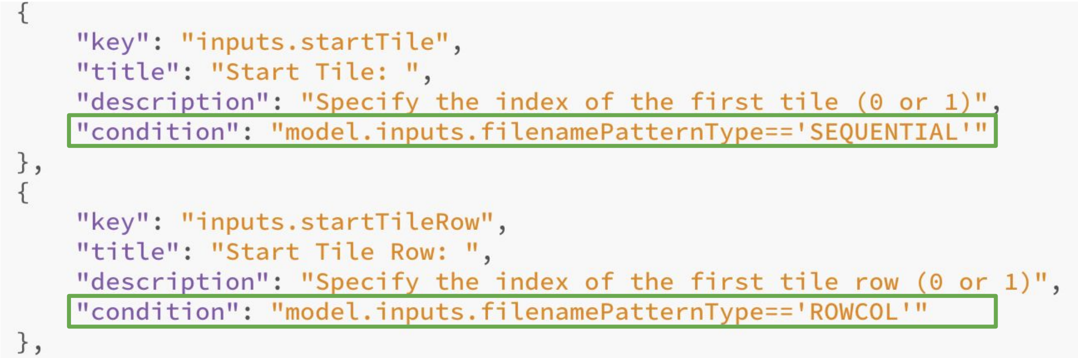
Threshold value:

FAIR-CCS manifest: UI section

Description of UI

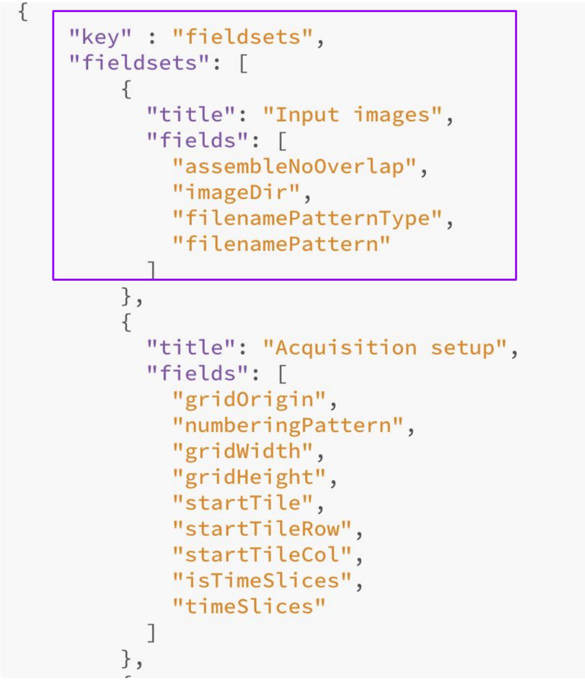
Example of more advanced UI options
(conditional visibility and fieldsets)

Conditional visibility of fields



```
{
    "key": "inputs.startTile",
    "title": "Start Tile: ",
    "description": "Specify the index of the first tile (0 or 1)",
    "condition": "model.inputs.filenamePatternType=='SEQUENTIAL'"
},
{
    "key": "inputs.startTileRow",
    "title": "Start Tile Row: ",
    "description": "Specify the index of the first tile row (0 or 1)",
    "condition": "model.inputs.filenamePatternType=='ROWCOL'"
},
```

Fieldsets

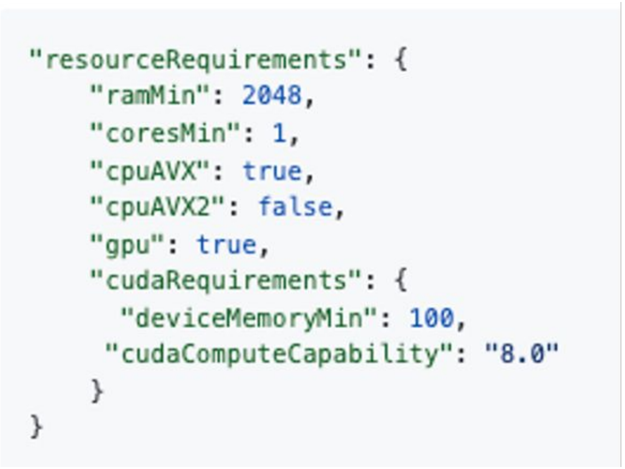


```
{
    "key" : "fieldsets",
    "fieldsets": [
        {
          "title": "Input images",
          "fields": [
            "assembleNoOverlap",
            "imageDir",
            "filenamePatternType",
            "filenamePattern"
          ]
        },
        {
          "title": "Acquisition setup",
          "fields": [
            "gridOrigin",
            "numberingPattern",
            "gridWidth",
            "gridHeight",
            "startTile",
            "startTileRow",
            "startTileCol",
            "isTimeSlices",
            "timeSlices"
          ]
        },
```

FAIR-CCS manifest: Resource requirements section

Resource/hardware requirements

- Optional
  - “ramMin”: minimum RAM in Mebibytes (Mi)
  - “coresMin”: minimum number of CPU cores
  - “cpuAVX”: Advanced Vector Extensions (AVX) CPU capability required
  - “cpuAVX2”: Advanced Vector Extensions (AVX) CPU capability required
  - “gpu”: GPU/accelerator required
  - “cudaRequirements”: GPU Cuda-related requirements
    - “deviceMemoryMin”: minimum device memory
    - “cudaComputeCapabilities”: single minimum value or array of valid values for required compute capability



```
"resourceRequirements": {
    "ramMin": 2048,
    "coresMin": 1,
    "cpuAVX": true,
    "cpuAVX2": false,
    "gpu": true,
    "cudaRequirements": {
      "deviceMemoryMin": 100,
     "cudaComputeCapability": "8.0"
    }
}
```

FAIR-CCS Github repository:

https://github.com/usnistgov/fair-chain-compute-container

Questions?

wipp-team@nist.gov