LA-UR-20-26061

Managing Dynamic Workflows in BEE

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BEE: Build and Execute Environment

- Goal: to create a unified software stack to *containerize* HPC apps
- Seeks to simplify execution of complex scientific workflows on HPC systems by:
  - Modeling workflows using a workflow language specification (CWL)
  - Storing and visualizing workflows as DAGs in a graph database (Neo4j)
  - Managing workflow execution using the BEE workflow engine
- Supports Charliecloud and Singularity containers
- Supports the Slurm workload manager

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HIGH PERFORMANCE COMPUTING

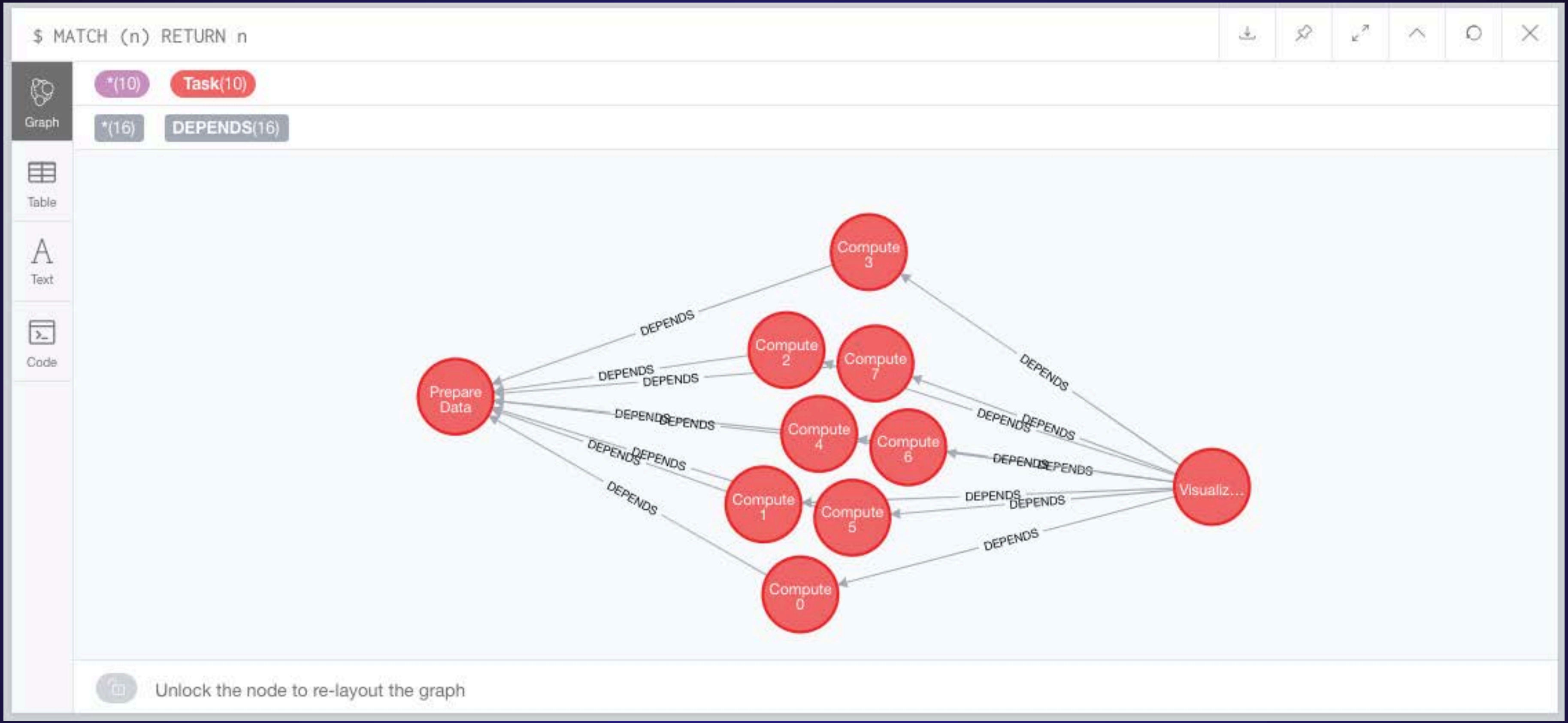
Motivation

- BEE seeks to support as much of CWL as possible
- Currently only supports workflows in which inputs and outputs between steps are known *a priori*
  - Not sufficient for complex dynamic workflows in which:
    - Unknown numbers of outputs may be generated by a step
    - A task may need to be run on each of them (scatter)
    - A subsequent step may depend on all of them as inputs (gather)
- The way BEE models workflows needs to change

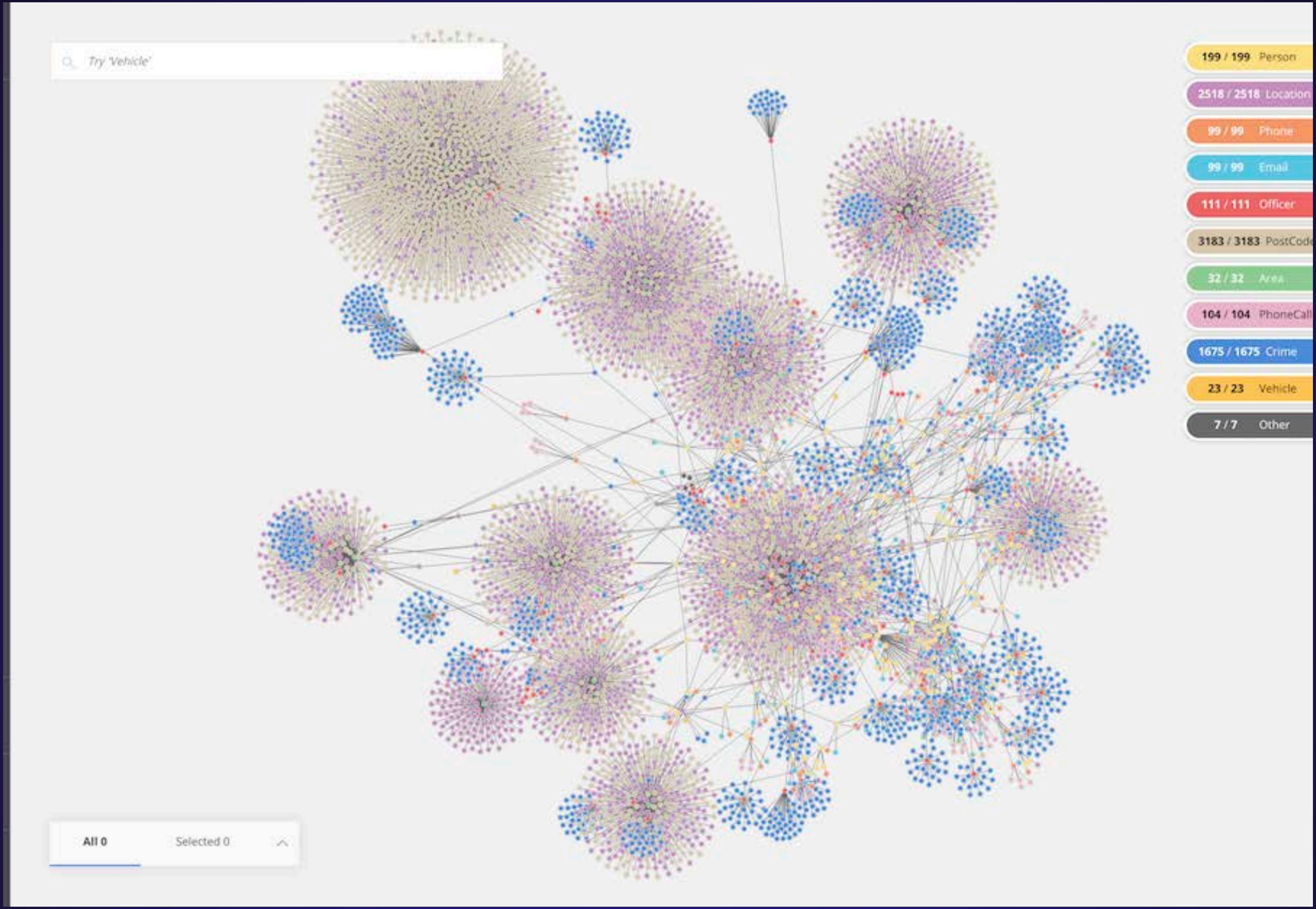
Neo4j and Cypher

- Neo4j
  - Transactional graph database
  - Stores data as nodes and relationships with properties
  - Uses the Cypher Query Language
  - Supports visualization of database in a browser
  - Extremely scalable
- Cypher
  - Declarative “SQL-inspired” query language
  - Visual and logical syntax
  - Example: get tasks dependent on a task given by `$task_id`

```
MATCH (t:Task)-[:DEPENDS]->(:Task {task_id: $task_id})
RETURN t
```

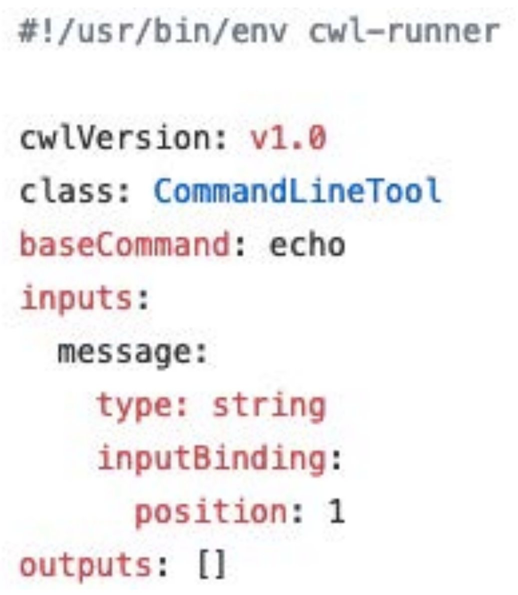


```
$ MATCH (n) RETURN n
```


Try 'Vehicle'
199 / 199 Person
2518 / 2518 Location
99 / 99 Phone
99 / 99 Email
111 / 111 Officer
3183 / 3183 PostCode
32 / 32 Area
104 / 104 PhoneCall
1675 / 1675 Crime
23 / 23 Vehicle
7 / 7 Other
All 0
Selected 0

CWL: Common Workflow Language

- An open standard for describing analysis workflows and tools
- Makes workflows portable and scalable
- Allows execution of workflows on a variety of HPC and cloud environments
- Specification syntax based on YAML
- Example: run the echo command on an input string



```
#!/usr/bin/env cwl-runner

cwlVersion: v1.0
class: CommandLineTool
baseCommand: echo
inputs:
  message:
    type: string
    inputBinding:
      position: 1
outputs: []
```

Former BEE Workflow Model

Former BEE Workflow Model – Data Structures

- Task
  - UUID
  - Name
  - Command
  - Hints
  - Subworkflow
  - Inputs
  - Outputs
  - State
- Metadata
  - Workflow Hints
  - Workflow Requirements

- Tasks are created and added to the graph database as nodes through the workflow interface
- Dependencies are modeled as DEPENDS_ON relationships between tasks, automatically created when tasks are added
  - Cypher query matches ins/outs
- Metadata node stores hints and requirements of workflow

Former BEE Workflow Model – Execution

- The workflow execution is initialized through the workflow manager
  - Workflow execution may also be paused or stopped through the WFM
- Task may execute when all of its input dependencies are satisfied
  - Requires all task inputs/outputs to be known prior to execution
  - Does not support complex dynamic workflows
- CWL supports task “scattering”
  - Task is specified to run multiple times over an array of inputs

Complex Dynamic Workflow

scatter.cwl (partial)

```
cwlVersion: v1.0
class: Workflow

requirements:
 ScatterFeatureRequirement: {}

inputs:
  experience_score: int
  interview_score: int
  test_score: int
  iterations: int
  datasetpath: string
outputs:
  final_answer:
    outputSource: predict/answer
    type: float
steps:
  read:
    run: /home/bee/cwl2/read.cwl
    in:
      x: datasetpath
    out:
      - output_array
  preprocess:
    run:/home/bee/cwl2/preprocess.cwl
    scatter: data_column_file
    in:
      x:read/output_array
    out:
      - output_preprocessed_array
```

read.cwl

```
cwlVersion: v1.0
class: CommandLineTool
baseCommand: ["python", "/home/bee/cwl2/finalread.py"]

inputs:
  x:
    type: string
    inputBinding:
      position: 1

stdout: output.txt

outputs:
  output:
    type:
      type: array
      items: File
    outputBinding:
      glob: "*.txt"
```

- Reads dataset and outputs data in each column as its own file
  - Number of columns unknown
- Scatters the output array for preprocessing

Complex Dynamic Workflow

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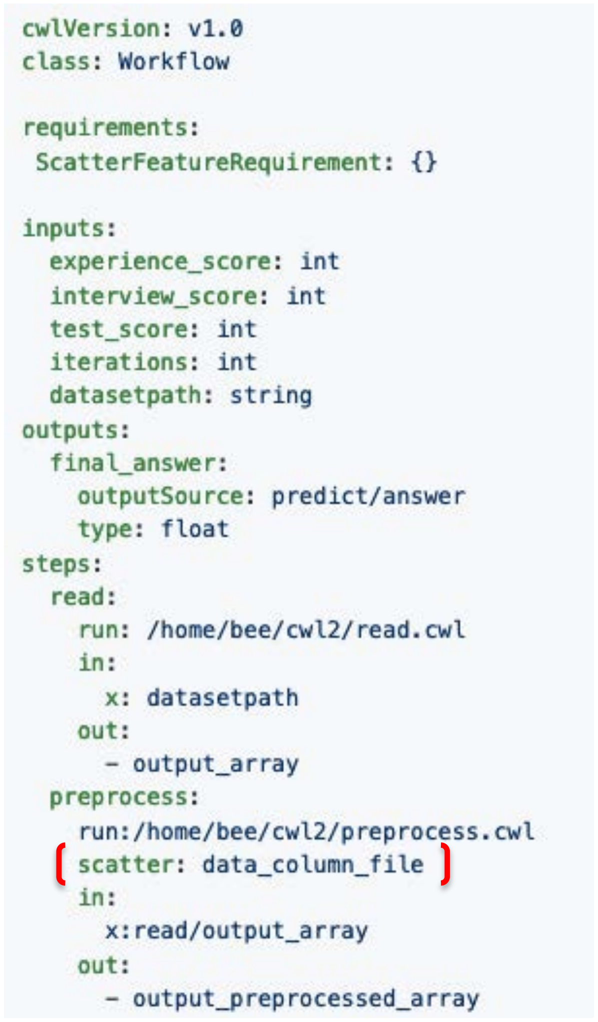

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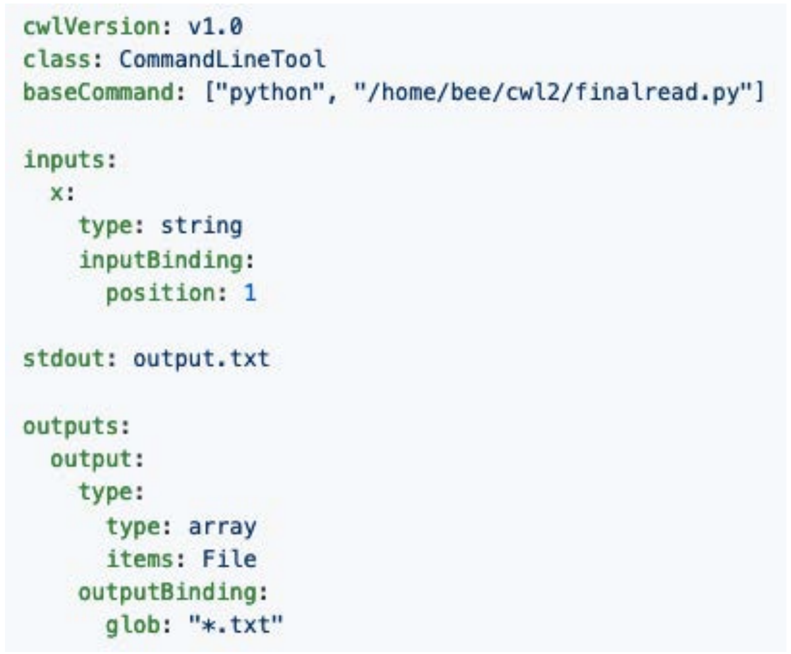

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HIGH PERFORMANCE COMPUTING

Updated BEE Workflow Model

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- Task
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  - Subworkflow
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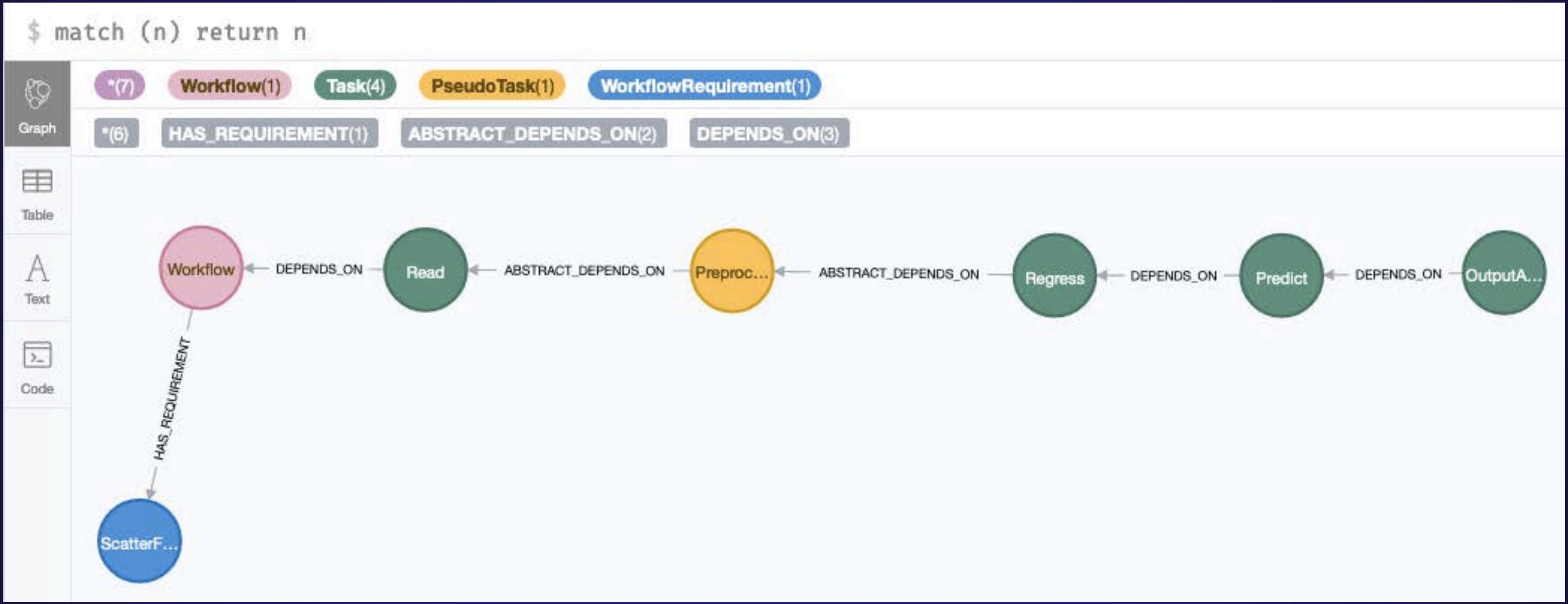
  - Outputs
  - State
- WorkflowHints
  - Hints
- WorkflowRequirements
  - Requirements
- TaskHints
  - Hints
- Tasks created/added through workflow interface
- Workflow node points to first task of workflow
- Hints and requirements stored in own nodes
  - Related to tasks and workflow by HAS_HINT and HAS_REQUIREMENT relationships
- Dependencies modeled by DEPENDS_ON relationships

Updated BEE Workflow Model – Pseudo-Tasks

- PseudoTask
  - UUID
  - Name
  - Command
  - Subworkflow
  - Abstract Inputs
  - Outputs

- PseudoTasks are created for tasks whose inputs are not known *a priori*
  - Dependency relations to and from PseudoTasks modeled as ABSTRACT_DEPENDS_ON relationships
  - Expand into as many tasks as required to handle each input
- Real outputs are returned to Workflow Manager to expand PseudoTasks



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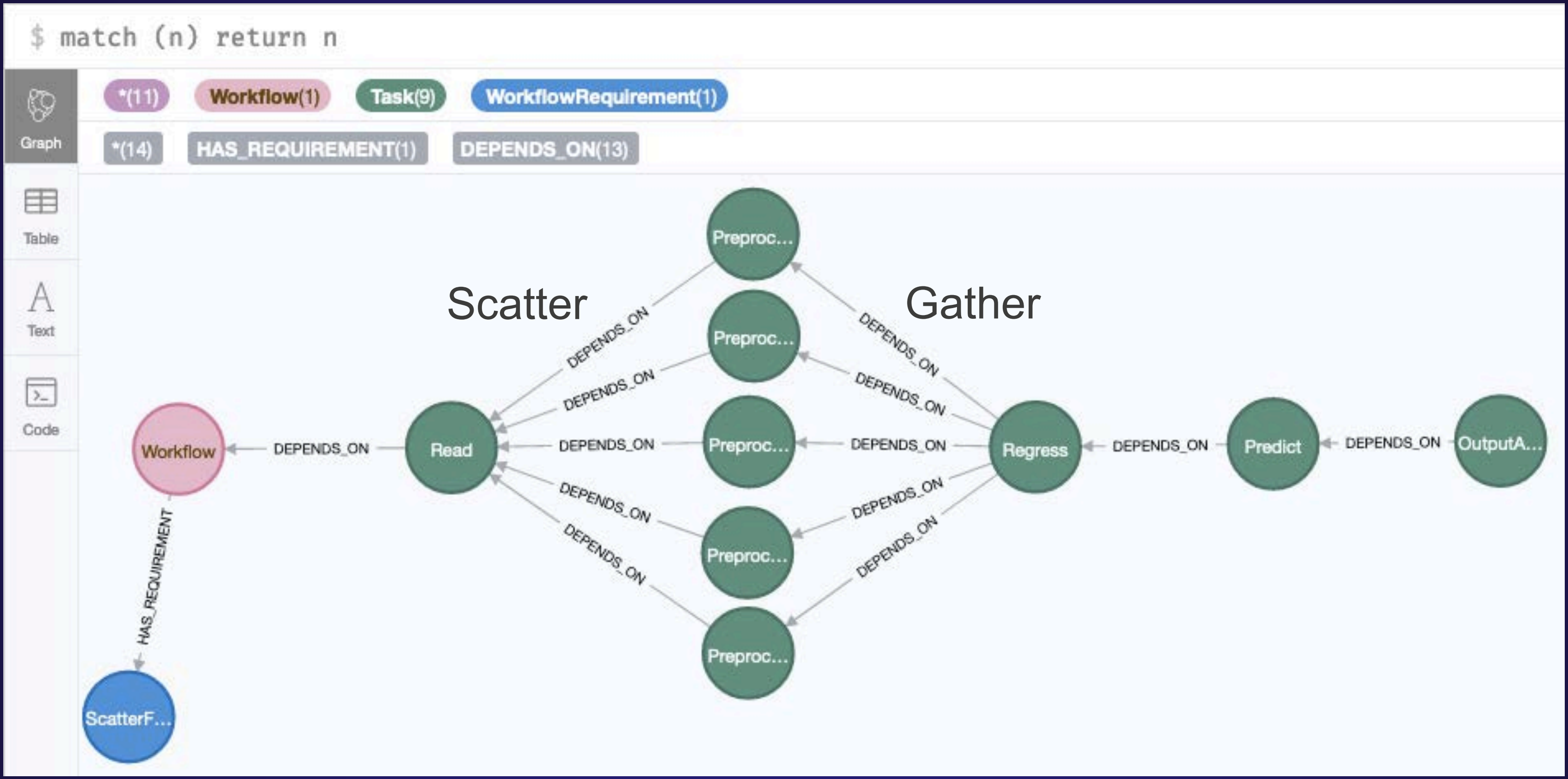

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Conclusion

- BEE is a powerful tool for:
  - Managing and visualizing scientific workflows
  - Simplifying workflow execution on HPC and cloud platforms
- BEE supports much of the CWL specification
- Did not support execution of complex ”scattering” workflows
- By introducing the PseudoTask:
  - Can generate tasks to run on variable number of inputs
  - BEE is another step closer to supporting the entire CWL specification
  - BEE can now support parallelized workflows with scattering tasks

Further Work

- Add support for embedded Javascript or Python expressions in CWL

- Add support for nested workflows in CWL

Questions?

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Over 70 years at the forefront of supercomputing