10 Dec 2024

- Review of proposed syntax changes (<u>pydra#766</u>)
- Roadmap to version 1
- Help with how the pydra.engine.state.State class works
- Publishing Pydra?

23 Apr 2024

- Explicit paths being copied and rewritten to workflow cache directory
 - Seems to be a bug
 - Linking/copying one node's cache directory outputs to another's seems fine, but
 Path should be respected
- Pydra support
 - Satra's group is the only one with funding for Pydra explicitly
 - Nipreps aiming to write new tools with Pydra tasks and nipype1 interfaces, to avoid continuing lock-in
 - Tom has an interface/

16 Apr 2024

- Points for discussion
 - o v0.23 released!
 - Ghislain is working through Clinica test suite
 - Nipype2pydra
 - Function task converter (<u>nipvpe2pvdra#13</u>)
 - Package layout (e.g. nipvpe/pvdra-ants@nipvpe-auto-conv)
 - Testing framework
 - Pytest structure
 - o Inputs tested with TimeoutWorker
 - Outputs tested from reference working dir
 - Reference data
 - o Detailed typing and Fileformats.sample() method
 - o Where to store it
 - Text-based workflow converter (i.e. regular expression based)
 - o Path to v1.0
 - Plans for picking up docs/tutorial work again (tutorial objectives)
 - Proposed syntax changes (#692)
 - Target % of nipype interfaces converted??
 - Improving the "sad path" experience
 - E.g. Crash Jupyter notebooks
 - ..

28 Feb 2024

- Points for discussion
 - o v0.23 release
 - Tom's outstanding PRs
 - Hash change guards #698
 - Caching of file-set hashes by local path and mtimes #700
 - Bugfix for optional output template files #709
 - BYO worker #733
 - Environments feature
 - How does it work?
 - Whether an "environment manager" would work (#701)
 - Anything else?
 - Nipype2pydra
 - Function task converter (<u>nipype2pydra#13</u>)
 - Package layout (e.g. <u>nipype/pydra-ants@nipype-auto-conv</u>)
 - Testing framework
 - Pytest structure
 - Inputs tested with TimeoutWorker
 - Outputs tested from reference working dir
 - Reference data
 - Detailed typing and Fileformats.sample() method
 - Where to store it
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 - Plans for picking up docs/tutorial work again (tutorial objectives)
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 - Improving the "sad path" experience
 - E.g. Crash Jupyter notebooks
 - ...

19 Sep 2023

- Points for discussion (link to related issues/PRs/etc)
 - Tom: Syntax changes proposal <u>pydra#692</u>
 - Using October "hack week" to focus on documentation/tutorials, preparing notes here
 - Environments <u>pydra#516</u>
 - What still needs to be done?
 - Tom: Would concept of "Environment Manager" work? pydra#701
 - Tom: PRs to finish off typing/hashing work
 - Caching file hashes by path+mtime: pydra#700
 - Hash change guards: pydra#698
 - Superclass auto cast: pydra#696
 - SLURM/dask-related test/coverage failures pydra#667

- Tom: Making Pydra a proper "namespace package" pydra#679
- Time of next meeting with daylight savings change (in Oz)
- Updates to the tutorial

Notes

- October hack week to focus on reworking documentation/tutorials
 - Syntax changes (such as <u>pydra#692</u>) could be proposed as part of this process
 - Look to what is done well (and not) in Nipype docs/tutorials
 - Use Diataxis approach for organising docs (https://diataxis.fr/)
 - Structure of docs to be revisited
 - Discussion on whether to combine docs and tutorial into one site/repo or keep separate
 - Use combination of JupyterBook for tutorials and potentially furo sphinx theme for conceptual/api reference
 - Online doc containing separate headers for 4 themes outlined in Diataxis to be circulated prior to hack week for brainstorming
- Next release
 - Aim to complete within a few weeks
 - To include typing/hashing and environment PRs listed above (<u>pydra#700</u>, <u>pydra#698</u>, <u>pydra#696</u>, <u>pydra#516</u>)
- Keep the same time for future meetings for October, but revisit when NH clocks go back in Nov

29 Aug 2023

- Points for discussion (link to related issues/PRs/etc)
 - Tom: Static type-checking: pydra#670, TLDR:
 - task definition syntax changes
 - wf syntax changes
 - task/wf execution changes
 - Satra's concerns and my response
 - Summary of bw-compat.-breaking syntax changes
 - Tom: Update on auto-gen of task packages for nipype2pydra conv: nipype2pydra:#10
 - "Backlog" (to be carried over but probably won't have time)
 - Tom: Intermittent failures gathering results with CF: pydra#671
 - Aditya: Slurm discussion: pydra#667
- Additional notes
 - Chris: Refactoring Environment PR
 - Dorota:
 - Updating tutorials to use type checking
 - Fixed dask!
 - Newer version of slurm container
 - o Tom:

- State of the issues/PRs:
 - #653 has a couple helper functions
 - #655 Changes tasks to dataclasses
 - #670 (issue) has broader discussion

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3 Aug 2023

- Points for discussion (link to related issues/PRs/etc)
 - Tom: Type checking PR: pydra#662
 - Relaxing type-checking for super classes: pydra:#682
 - Guards on task hashes changing during execution: <u>pydra:#681</u>
 - Upper-bounding fileformats dependency
 - Docs failing
 - Splitting of nodes in inner workflows no longer supported
 - Caching of file-hashes no longer performed pydra:#683
 - Tom: Auto-gen of task packages for nipype2pydra conv: nipype2pydra:#10
 - Tom: Intermittent failures gathering results with CF: <u>pydra#671</u>
 - o Tom: Static type-checking: pydra#670, TLDR:
 - task definition syntax changes
 - wf syntax changes
 - task/wf execution changes
 - Satra's concerns and my response
 - Aditya: Slurm discussion: pydra#667
- Additional notes
 - Typing PR (pydra#662) merge accepted, to be released as an alpha for now
 - <u>pydra:#682</u>, <u>pydra:#681</u>, <u>pydra:#683</u> accepted in principle, will look to implement before full release
 - Upper-bounding fileformats dependency rejected due to bad experience doing this with Nipype
 - Docs failing due to sphinx update
 - Splitting of nodes in inner workflows functionality dropped (and test deleted) because it doesn't have a strong use case
 - Auto-gen of task packages (<u>nipype2pydra:#10</u>) for nipype2pydra accepted in principle:
 - Test out how it works for a few toolkits (I was thinking ANTs, AFNI and FSL) before moving on to generate repositories for all nipype interface subpackages
 - Static type-checking (<u>pydra#670</u>) to be discussed in the next dev meeting

29 June 2023

Points for discussion (link to related issues/PRs/etc)

Tom: Type checking PR: pydra#662

Ghis: Lazy field in template PR: pydra#657

Yibei: Converter nipype2pydra: nipype2pydra#6

Aditya: Slurm discussion: pydra#667

o Tom: Intermittent failures gathering results: pydra#671

Tom: Static type-checking: pydra#670

Tom: min/max field values (are they supported?)

Additional notes

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23 May 2023

- Discussion notes
 - Introductions (welcome, Aditya!)
 - GSoC proposal: <u>link</u>
 - Possible topics (late breaking agenda)
 - BIDS-Prov: BIDS Extension Proposal (BEP028): Provenance
 - File hashing
 - Debugging
 - Tom's suggestion for Jupyter notebook reconstructing path to allow interactive inspection
 - Maybe a dashboard based on the audit interface could cover much of this use case? This was a previous idea of Satra's.
 - File hashing / input coercion
 - Tom: Coerce file-likes and basic containers (lists, dicts, sets), otherwise leave inputs alone
 - Need to consider map/combine-related (nested) lists
 - LazyInputs/Outputs should have type tags (need not be proper Python annotations) so we can check connection validity without values

Table for the meetings week 2

Topics for meeting / hacking in week 2	People interested in working	Additional people for discussion	Meeting time: week2 In EDT (Boston)
General updates	DJ, YC, GV, TC, CM		8-8:30 Tuesday (DJ, GV, TC, CM)
Updates for autoconverter to	DJ, YC, GV, TC		12-13 Tue (DJ+YC)

translate the interfaces			8-9 Wed (DJ, GV, TC)
Workflow provenance	DJ, TC	SG (?)	
Input/output convention updates	GV, CM, DJ, TC		8:30-9:00 Tuesday (DJ, GV, TC, CM)
Hash dispatch updates plus file format Integration	TC, DJ, CM		
File manipulation task: datalad (?)	DJ, YC	YH (?)	
File manipulation: fsspec types exploration (?)	СМ		

Topics	People interested in working	Additional people for discussion	Weeks: week1 (May 2nd, 3d), week 2 (May 9th, 10th)	Meeting time: week1 In EDT (Boston)
Using autoconverter to translate the interfaces	DJ, YC, GV, TC		week 1	Tue 8-9am (DJ, GV, TC); Tue 10:30-11:00 am: updates for Yibei (DJ, YC)
Workflow provenance	DJ, TC	MD (?) - no answer	Week 2	
SPM matlab	DJ, GV, CM(?),	SG (?) - Satra in DC	Week 1	Tue 9am (DJ, GV, CM)
Input/output	GV, CM, DJ,		Week 1	Wed 8-9am (GV,

convention	TC(?)			CM, DJ, TC)
Hash dispatch	CM, TC		Week1	Tue 4:30-5:00 (CM, TC)
File format Integration	TC, DJ,		Week 2	
File manipulation task: datalad	DJ, YC	YH (?)	Week 2	
File manipulation: fsspec types exploration	СМ		Week 2	
IPython notebook "crashfile"	тс		Week 2	

Hack Days: May 2023

Discussion about File/Directory

- Why do we need it:
 - Hashing
 - Containers
 - validation that exists
- Finishing Environment class first 516
- Finishing hashing: 644
- For type checking:
 - File = ty.NewType("File", Path)
 This probably will not work
 - Alias this is probably the way to go
- Internally we will be using Path-like
- In the future we should allow for more specific formats (Tom's package) that would provide some extra validation

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Converter meeting:

Tom's generic converter repo (not tested yet):
 https://github.com/Australian-Imaging-Service/nipype2pydra

Tom was pretty convinced that we can build generic converter after working with several packages:

- Ants converter:
 https://github.com/tclose/pydra-ants/blob/port-converter/tools/converter.py
- Freesurfer:
 https://github.com/ablachair/pydra-freesurfer/blob/port-converter/tools/converter.p
 v
- Issues with converter:
 - Naming convention:
- Example from Ghislain: interfaces converted manually:
 - Harder since I dodn't use the nipype as a starting points
 https://github.com/aramis-lab/pydra-freesurfer/blob/main/src/pydra/tasks/freesurfer/gtmseg.py
 - https://github.com/aramis-lab/pydra-fsl/blob/main/src/pydra/tasks/fsl/eddy.py
 - https://github.com/aramis-lab/pydra-fsl/tree/main/src/pydra/tasks/fsl/utils

SPM meeting:

Drop MCR vs Matlab distinctions in-task

March 2023

Hackday: May 2-3rd, May 9-10th (Tuesday, Wednesday)

Todo before/during hack day:

- Pydra-fsl moved to nipype and update metadata
 - Test autoconverter and prepare the summary of the issues (DJ +YC will try to test before)
- The same for pydra-freesurfer
- Logging

- Workflow Provenance
 - Summary what was done by the Ryan and what is in the BIDS-Prov
- The SPM-task class (Satra for a meeting, discussion before the meeting)
- Naming of the input/output, perhaps some consistency among tools
 - Example for fsl/freesurfer from Ghislain (prepare a doc)
- File manipulation tasks
 - Pydra-datalad
 - DVC: https://dvc.org/
 - Basic data writing/reading, similar to DataGrabber; dynamic?
 - fsspec: https://filesystem-spec.readthedocs.io/en/latest/
- File format integration from Tom's package
- Reimplementation interface hashing using functools.singledispatch a la https://github.com/nipype/pydra/issues/626 (could be included in point above)

February 2023

discussion from Tom:

https://github.com/nipype/pydra/discussions/620#discussioncomment-5125962

- Yes, enable 'attrs'
- When define file in pydra; file=path-like, path-like + hash; intersection()
- Using mypy
- Pydra-fsl in PyPl
 - Plan when & how release (policy)
 - Lack of mechanisms of registrating plug-ins...
 - semi-auto-converter new name space?
 - Longer-descriptive name
 - Annotate xxx correspond to yyy in nipype (either in yml or code)
 - Combine ghislain's fsl package with pydra-fsl (did I miss anything here)
 - Add ghislain's fsl to pydra-fsl to see whether it can auto-converted
 - Keep the history how the task was developed/maintained; dependency problem
- New syntax for Docker tasks (env class), ask for feedback:
 https://github.com/nipype/pydra/blob/rf/environments/pydra/engine/tests/test_dockertask.py#L35
- GSoC:
 - https://neurostars.org/t/gsoc-2023-project-idea-16-2-converting-existing-scientific-workflows-to-new-dataflow-engine-written-in-python-pydra-350-h/24593/4
 - https://neurostars.org/t/gsoc-2023-project-idea-16-1-adding-new-workers-and-res-ource-management-to-new-dataflow-engine-written-in-python-pydra-175-h/24592/8

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TO DISCUSS (for the future meeting):

- Dynamical workflow connections
 - Doing type-checking when constructing the workflow
 - Type-checking when people use pydra to construct their workflows
- Decision on name space (pydra hackathon late April & early May, Dorota will start a poll on github)

January 2023

- Fileformat: https://arcanaframework.github.io/fileformats/index.html
- Converting types
- New environment class: syntax for Docker:
 https://github.com/nipype/pydra/blob/493071d17fa3d069ff74cb7b9a4904ef4eb82
 3c2/pydra/engine/tests/test_dockertask.py#L35

November 2022

- Pydra tasks packaging:
 - https://github.com/nipype/pydra/issues/582
- Testing patterns
 - Doctests for cmdline generation (a la nipype 1)
 - '--dry-run' for tools that support it?
- Handling multiple versions of underlying tools
 - Old style: min/max_ver in input spec, state machine code in _list_outputs
 - Possibilities:
 - Separate packages: pydra-fsl5 and pydra-fsl6
 - Submodules: pydra.tasks.fsl.ver5, pydra.tasks.fsl.ver6, pydra.tasks.fsl.latest
 - Some level of min/max_ver still kept?
 - Considerations
 - Workflows written agnostic to underlying tools
 - Some overlaps with provenance...