



# Agenda

- What is CUDA and the CUDA Toolkit?
- Conda, channels, and how they're used to create a CUDA Toolkit environment
- The initial CUDA Toolkit conda packaging
  - ...and some of its problems
- The new CUDA Toolkit conda packaging!
  - ...and how you can take advantage of it as a package maintainer, end user, etc.
- Current status
- Next steps



#### What is CUDA and the CUDA Toolkit?

- Compute Unified Device Architecture (CUDA)
  - System drivers for programmable NVIDIA GPUs
- CUDA Toolkit (CTK)
  - GPU Accelerated Scientific Programming Libraries
  - NVCC (Compiler)
  - Cuda-GDB (Debugger)
  - Debug tools (Nsight, profiles, etc.)
  - cuBLAS, other libs, etc.





#### Conda

- Package manager (particularly in the Python & Data Science space)
- Language agnostic (so easy to glue C/C++ libraries, Python, Rust, Go, etc. together)
- User friendly (can install in user's home directory or elsewhere without issues)





#### **Conda channels**

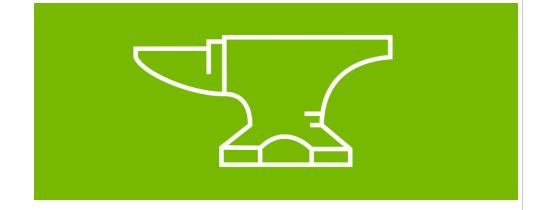
- Way to distribute a collection of packages that work together
- Similar to repos in Enterprise Linux
- Couple major ones and a few domain specific ones
- A few common Conda channels are...
  - defaults
  - conda-forge
  - nvidia
- Some domain specific ones:
  - rapidsai (data science libraries)
  - numba (particular for RC / nightlies of Numba)
  - dask (also for RC / nightlies)
  - pytorch (channel for pytorch + friends)

\$ conda install --channel conda-forge scipy



#### **Conda Channel Tiers**

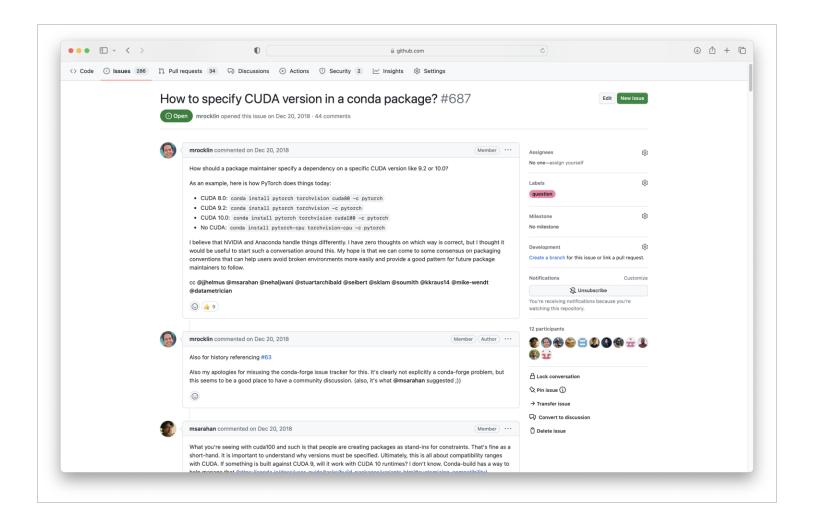
- Defaults
  - Professionally curated, self-contained, tested set of packages
- Conda-forge
  - Maintained by a community of packaging enthusiasts
  - Consumed by a broad range of users
  - Free to use / contribute to
  - Easily accessible / used without restrictions
  - Self-contained
  - Has lightweight installers for getting started
- Nvidia
  - Not quite as big as defaults & much smaller than conda-forge
  - Primarily CTK packages
  - Other packages: NVTabular, Merlin, cuQuantum, & some RAPIDS primitive libraries





## Initial versions and early cross-channel CUDA coordination

https://github.com/conda-forge/conda-forge.github.io/issues/687





## **CUDA Toolkit alignment**

#### For versions from 2018-present

- Align on cudatoolkit package for configuring CUDA version used by packages
- All CUDA packages depend on cudatoolkit
- Add \_\_cuda virtual package to Conda for CUDA driver support version detection
- Constrain cudatoolkit on \_\_cuda
- Recipe authors only need to think about adding `{{ compiler("cuda") }}` in `requirements/build`

### nvcc-feedstock meta.yaml

```
run_exports:
    strong:
{% if cuda_major_minor < (11, 2) %}
    - cudatoolkit {{ cuda_compiler_version }} {{ cuda_compiler_version }}.*

{% else %}
    - cudatoolkit >={{ cuda_compiler_version }},<{{ cuda_major + 1 }}

{% endif %}</pre>
```

### cudatoolkit meta.yaml

```
run_constrained:
{% if major_version < 11 %}
   - __cuda >={{ major_minor }}
{% else %}
   - __cuda >={{ major_version }}
{% endif %}
   - arm-variant * {{ arm variant type }}
```



### **CUDA Toolkit contents**

#### For versions from 2018-present in conda-forge

|--|--|--|



# So we are done right?

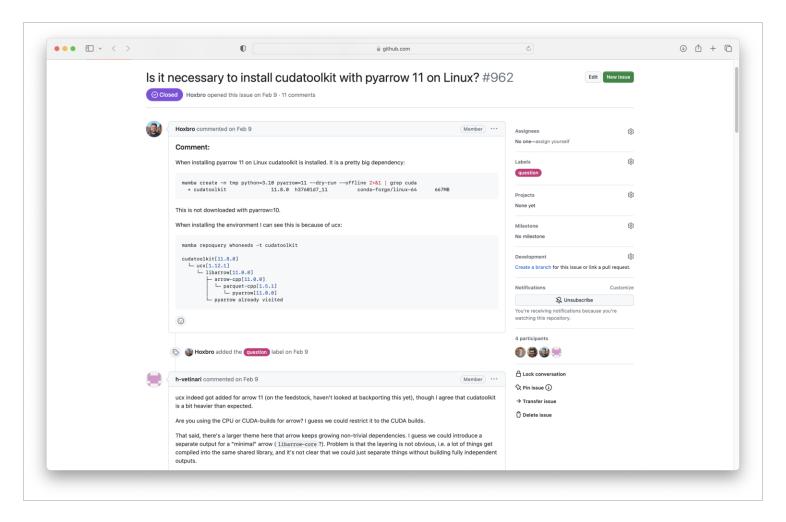
#### Excerpt from an "Odd Lots" Podcast episode

•	(Tracy Alloway) It seems with these large-scale systems that there's always change. Something is always in motion. Something is always in flux. Why is that?
•	(Patrick McKenzie) Well software engineers are working this week on a increasingly complex world where software is more leveraged than it had been even last week where there are increasing demands on the world etc Is there going to be a time where the last line of software is written? Probably not. There will never be a last bit of software writtenHumans want more things out of the world and we haveinfinite capacity for want at the margin.



#### cudatoolkit is massive!

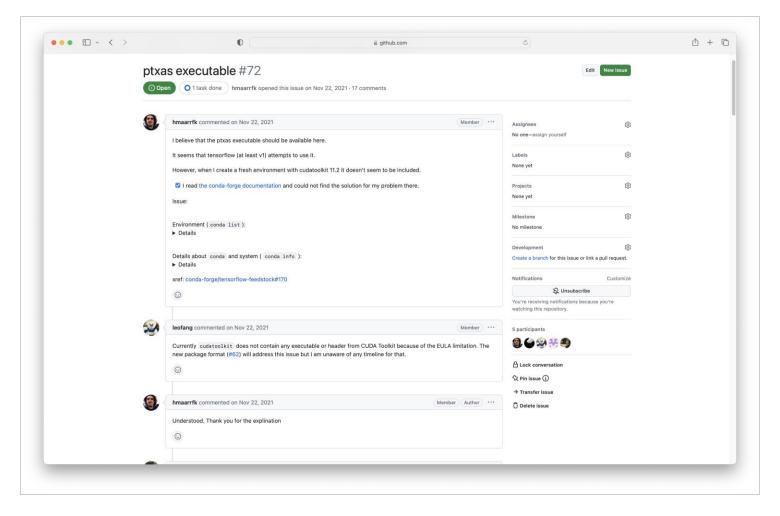
Is it necessary to install cudatoolkit with pyarrow 11 on Linux?





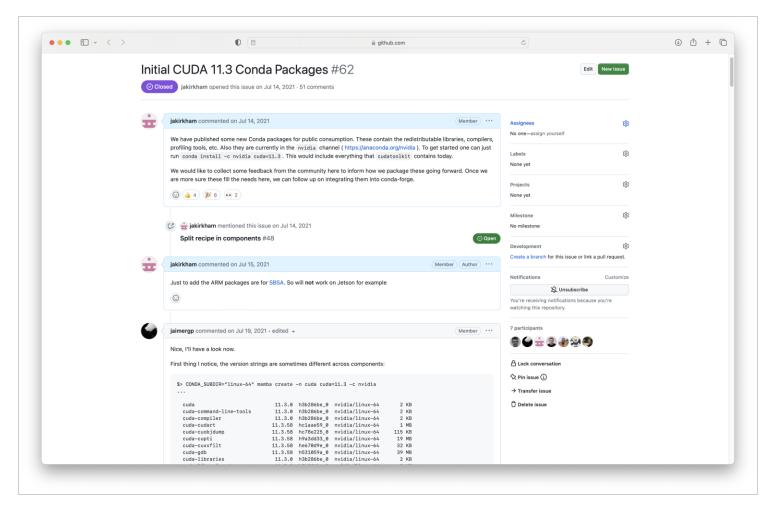
# And yet cudatoolkit is missing things?

ptxas executable (needed for tensorflow)



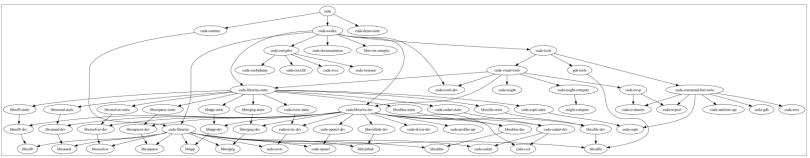
## Restructuring CTK packaging (in nvidia channel to start)

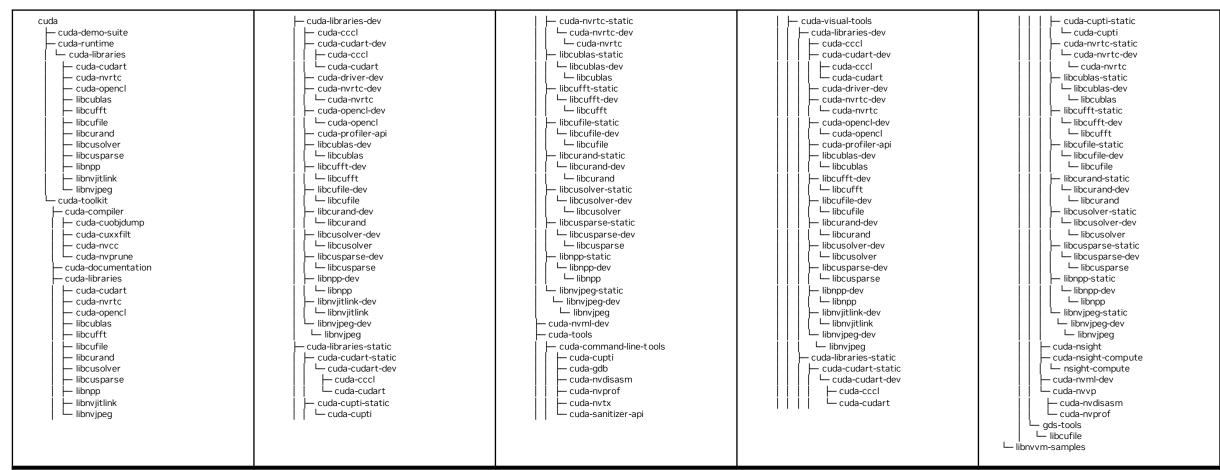
#### Initial CUDA 11.3 nvidia channel conda packages





## Restructuring CTK packaging





## CUDA Toolkit alignment

#### For upcoming CUDA 12 versions and newer

- Align on cuda-version package for configuring CUDA version used by packages (supersedes cudatoolkit)
- All CUDA 12 built packages depend on cuda-version
- CUDA 11 built packages using cudatoolkit can be constrained via cuda-version
- The cuda-version package is constrained by \_\_cuda virtual package (and cudatoolkit for legacy CUDA 11 support)
- Recipe authors still only need to think about adding `{{ compiler("cuda") }}` in `requirements/build`



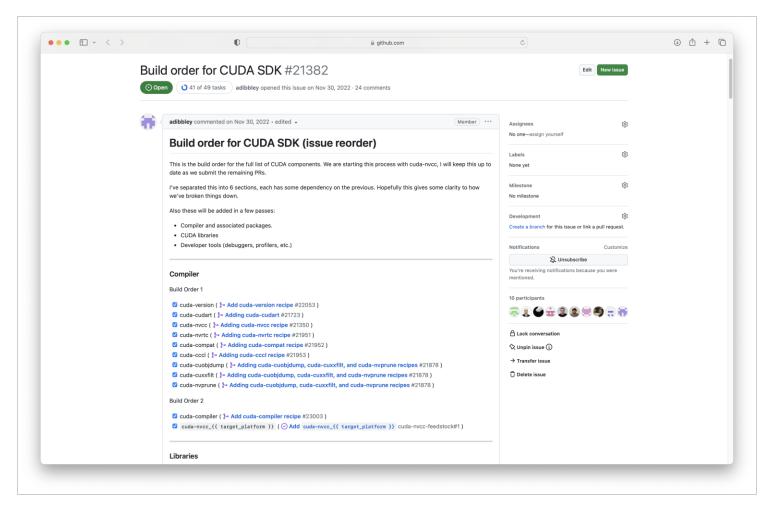
## **CUDA Toolkit alignment**

#### For upcoming CUDA 12 versions and newer

```
number: 1
                                                                                       number: 2
 skip: true # [(not linux) or (cuda_compiler_version !== "11.2")]
                                                                                       skip: true # [(not linux) or (cuda_compiler_version not in ("11.2",
                                                                                     "12.0"))]
 script: {{ PYTHON }} -m pip install . --no-deps -vv
                                                                                       script: {{ PYTHON }} -m pip install . --no-deps -vv
 missing_dso_whitelist:
                                                                                       missing_dso_whitelist:
   - '*/libcuda.*' # [linux]
                                                                                         - '*/libcuda.*' # [linux]
@@ -30,10 +30,15 @@ requirements:
                                                                                         - pip
    - pip
   - pybind11
                                                                                         - pybind11
   - python
                                                                                          - python
                                                                                         - cuda-cudart-dev # [(cuda_compiler_version or "").startswith("12")]
                                                                               33 +
                                                                                                            # [(cuda_compiler_version or "").startswith("12")]
                                                                               34 +
                                                                                          - libcublas-dev
                                                                                         - libcusparse-dev # [(cuda compiler version or "").startswith("12")]
                                                                               35 +
                                                                                leofang marked this conversation as resolved.
                                                                                                                                                · Show resolved
                                                                               36 +
                                                                                         - cuda-version {{ cuda compiler version }}
                                                                                       run:
 run:
   - {{ pin_compatible('custatevec', max_pin='x') }}
                                                                                         - {{ pin_compatible('custatevec', max_pin='x') }}
   - pennylane >=0.28
                                                                                         - pennylane >=0.28
   - python
                                                                                         - python
                                                                                          - {{ pin_compatible("cuda-version", min_pin="x", max_pin="x") }}
                                                                               41 +
test:
                                                                                     test:
```

## Current state: adding the new CTK CUDA 12.0 packages to conda-forge

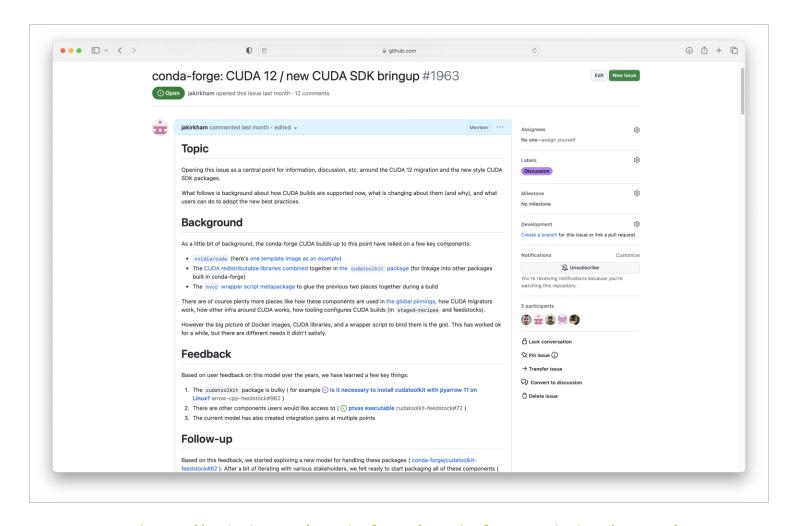
#### Build order for CUDA SDK





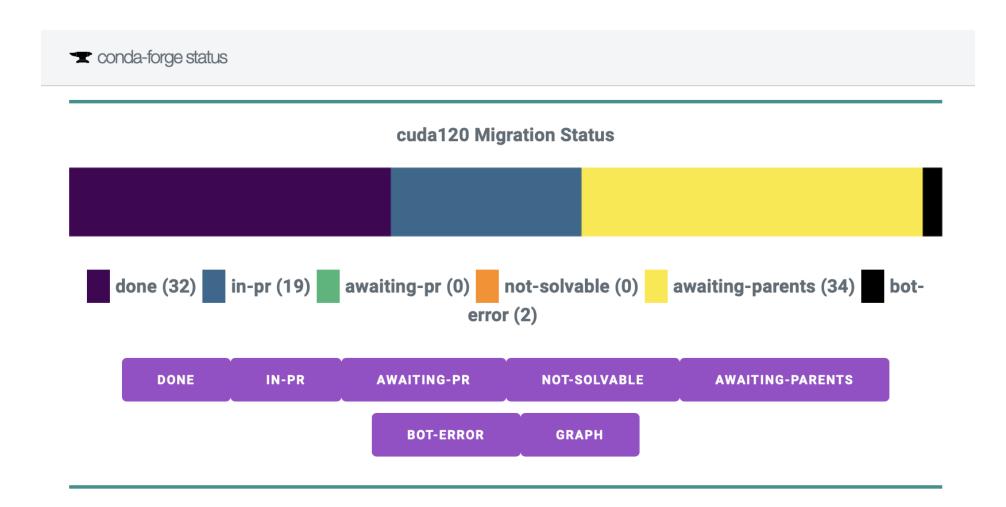
## Rebuilding of conda-forge packages with new CTK

conda-forge: CUDA 12 / new SDK bringup



## Conda-forge CUDA 12 migration

https://conda-forge.org/status/#cuda120





## Next steps

- Close out CUDA 12 migration
- Add new conda-forge CUDA documentation
- Update CTK packages for CUDA 12.1+
- Collect user feedback
- Evaluate next steps





Thank you!

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