

# PSICON 2020

LORI A. BURNS

PSICON 2020, BLUEJEANS

3-5 DECEMBER 2020





# ACQUIRING PSI4

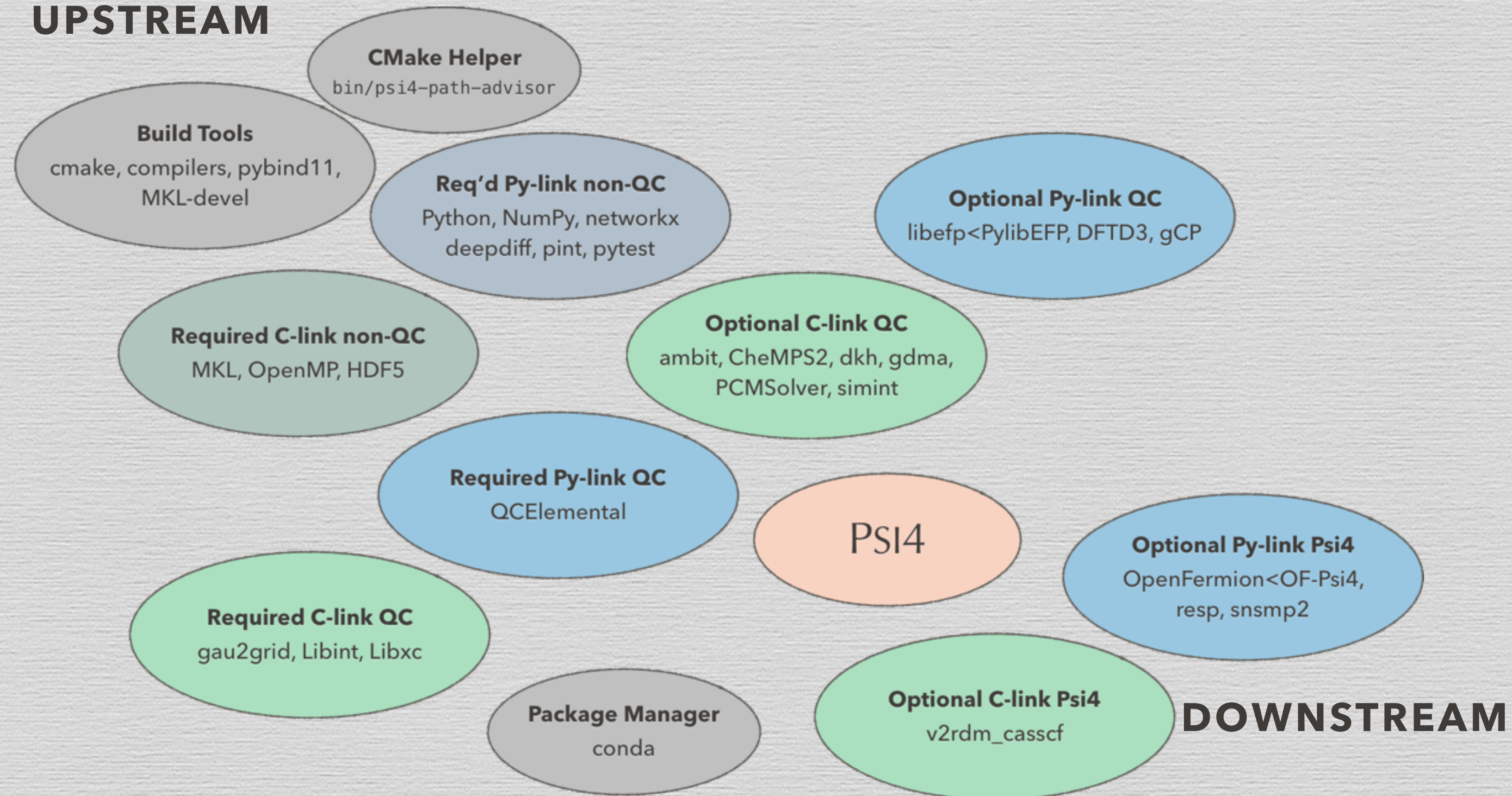
[psicode.org/downloads](https://psicode.org/downloads)



# ACQUIRING PSI4

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## UPSTREAM

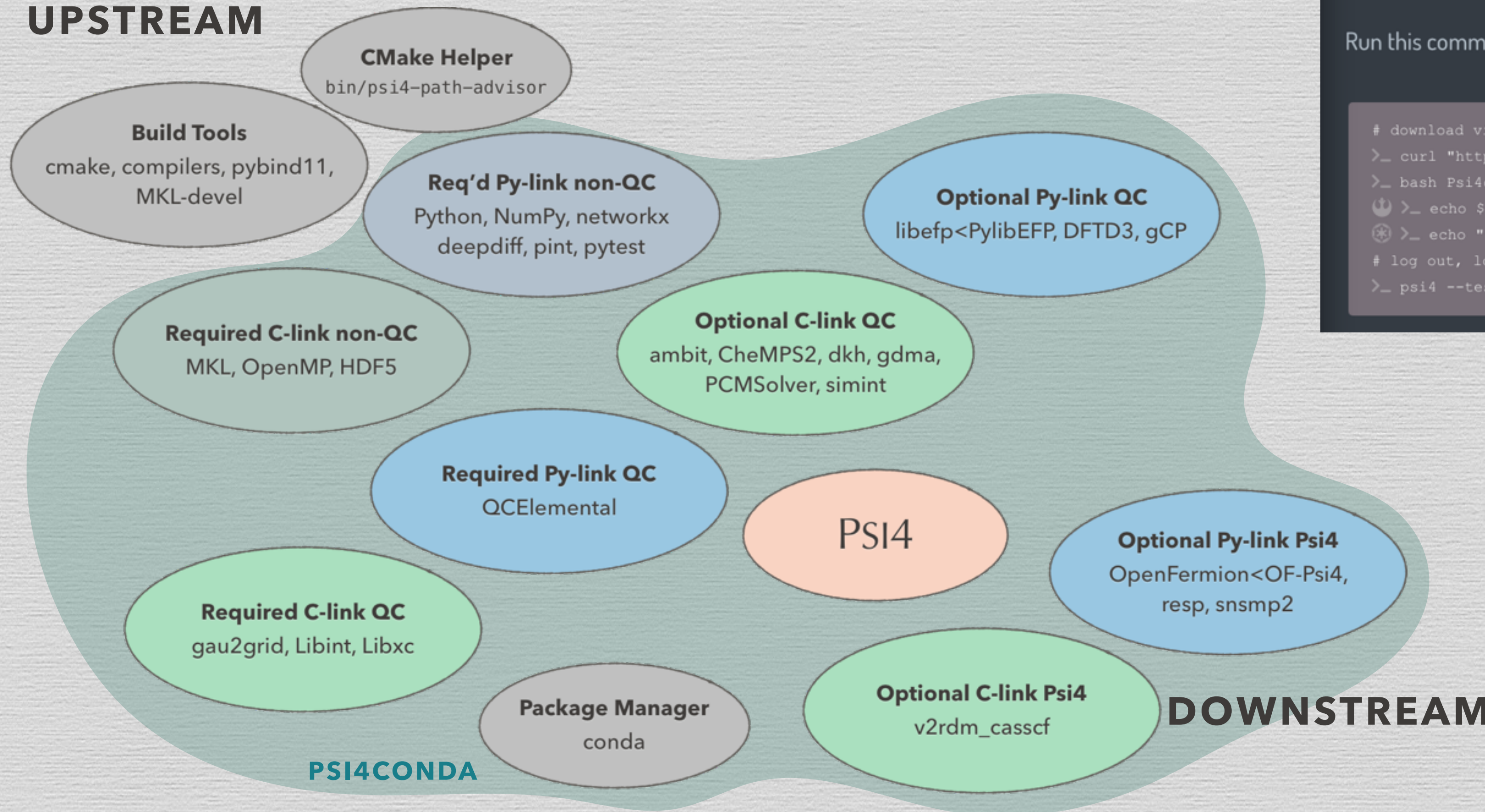




# ACQUIRING PSI4

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## UPSTREAM



## DOWNSTREAM

## Get Started with Psi4

### Select Preferences

<input checked="" type="checkbox"/> LINUX	<input type="checkbox"/> MACOS	<input type="checkbox"/> WINDOWS WSL	
<input checked="" type="checkbox"/> INSTALLER	<input type="checkbox"/> CONDA	<input type="checkbox"/> SOURCE	
<input type="checkbox"/> 2.7	<input type="checkbox"/> 3.5	<input type="checkbox"/> 3.6	<input checked="" type="checkbox"/> 3.7
<input type="checkbox"/> PREV RELEASE, v1.2.1	<input checked="" type="checkbox"/> STABLE RELEASE, v1.3	<input type="checkbox"/> NIGHTLY BUILD	

⚠ 64-bit; glibc 2.12 or higher. 🍏 64-bit; OS X 10.9 or higher. 🖥 64-bit; Windows Subsystem for Linux. 📄 Download standalone command-line installer. ● Use conda package manager. </> Build from source using tools and dependencies from conda. 🐍 Python included so choose the version you *want*, regardless of any you *have*.

### Run this command

📄 DOWNLOAD PSI4CONDA INSTALLER

```
# download via button above -OR- following line
>_ curl "http://vergil.chemistry.gatech.edu/psicode-download/Psi4conda-1.3-py37-Linux-x86_64.sh" -o
>_ bash Psi4conda-1.3-py37-Linux-x86_64.sh -b -p $HOME/psi4conda
📄 >_ echo $'. $HOME/psi4conda/etc/profile.d/conda.sh\nconda activate' >> ~/.bashrc
🌟 >_ echo "source $HOME/psi4conda/etc/profile.d/conda.csh\nconda activate" >> ~/.tcshrc
# log out, log back in so conda and psi4 in path
>_ psi4 --test
```

**PY-WARY USERS:**  
**CONDA INSTALLER**

Psi4 · dependencies · add-ons

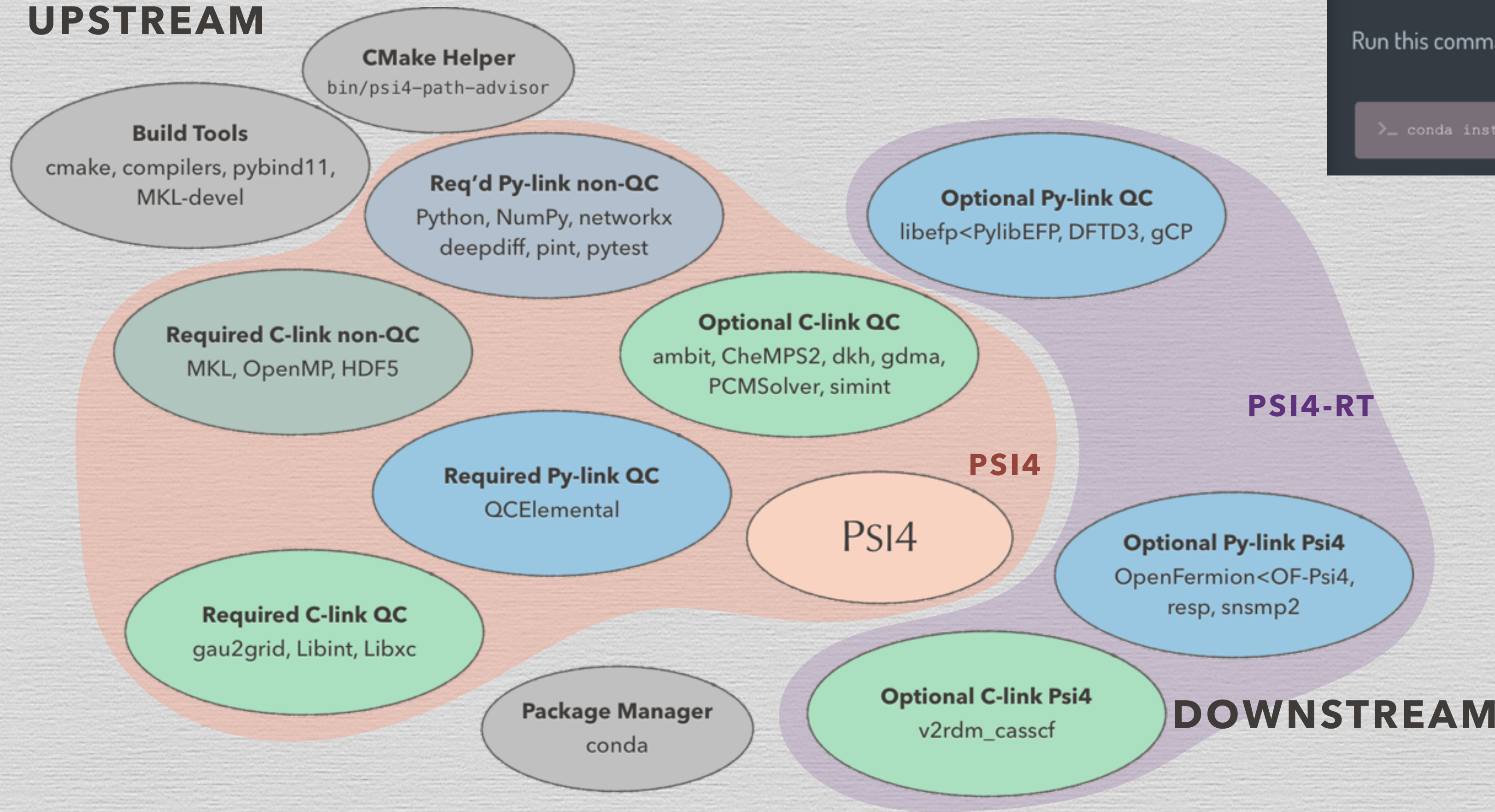
PSI4CONDA



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## UPSTREAM



## Get Started with PSI4

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### Run this command

[GOTO MINICONDA INSTALLERS](#)

```
>_ conda install psi4 psi4-rt python=3.7 -c psi4
```

## PY-FRIENDLY USERS: CONDA PACKAGE

PSI4 · dependencies · add-ons

## PY-WARY USERS: CONDA INSTALLER

PSI4 · dependencies · add-ons

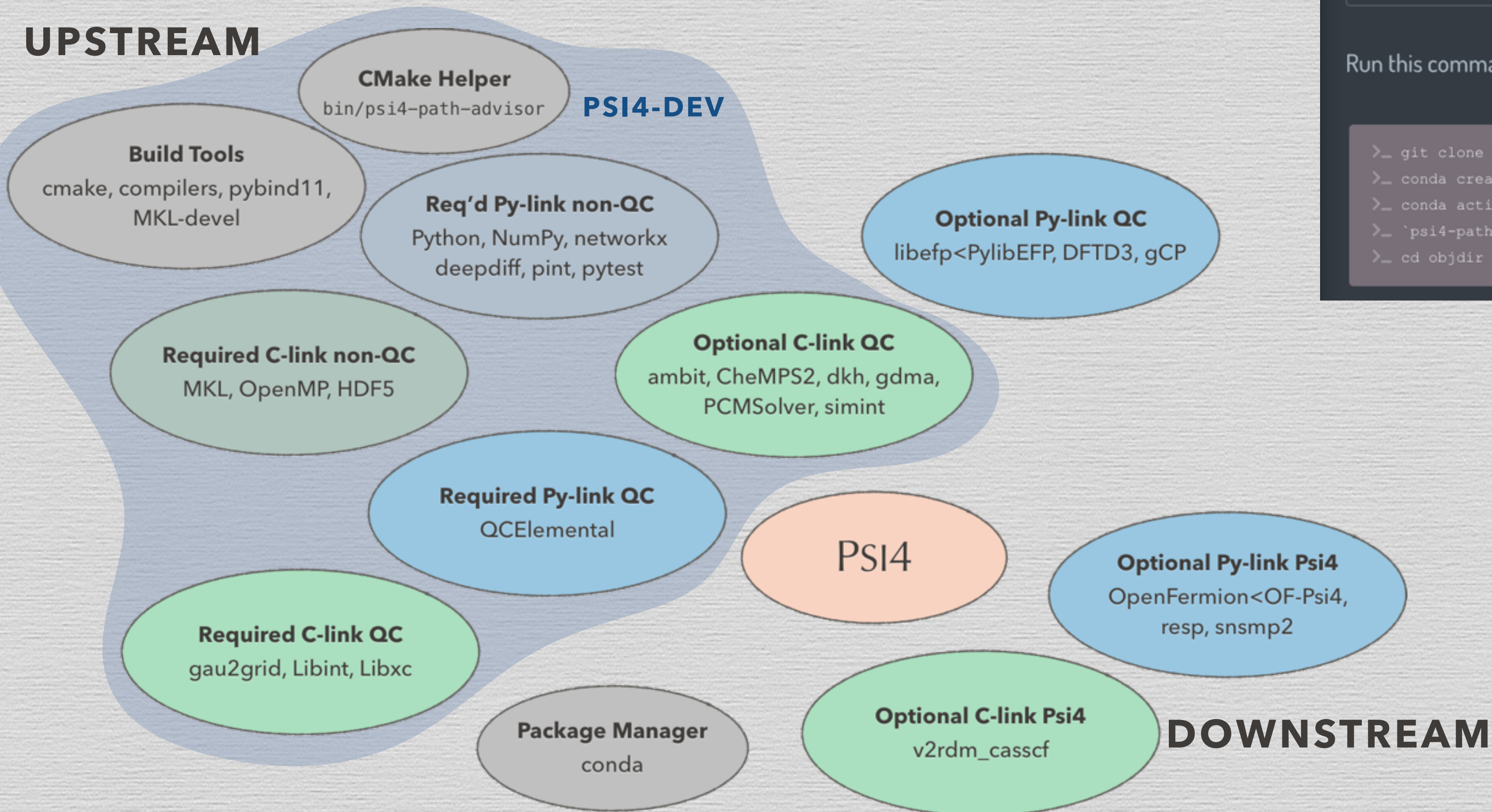
PSI4CONDA



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## UPSTREAM



## DOWNSTREAM

## Get Started with Psi4

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### Run this command

[GOTO MINICONDA INSTALLERS](#)

```
>_ git clone https://github.com/psi4/psi4.git && cd psi4
>_ conda create -n p4dev psi4-dev python=3.7 -c psi4/label/dev
>_ conda activate p4dev
>_ 'psi4-path-advisor --gcc'
>_ cd objdir && make -j`getconf _NPROCESSORS_ONLN`
```

## CORE DEVELOPERS: CONDA-ENABLED SUPERBUILD

deps · dev tools · add-ons · cmake hints

## PY-FRIENDLY USERS: CONDA PACKAGE

PSi4 · dependencies · add-ons

## PY-WARY USERS: CONDA INSTALLER

PSi4 · dependencies · add-ons

PSI4CONDA

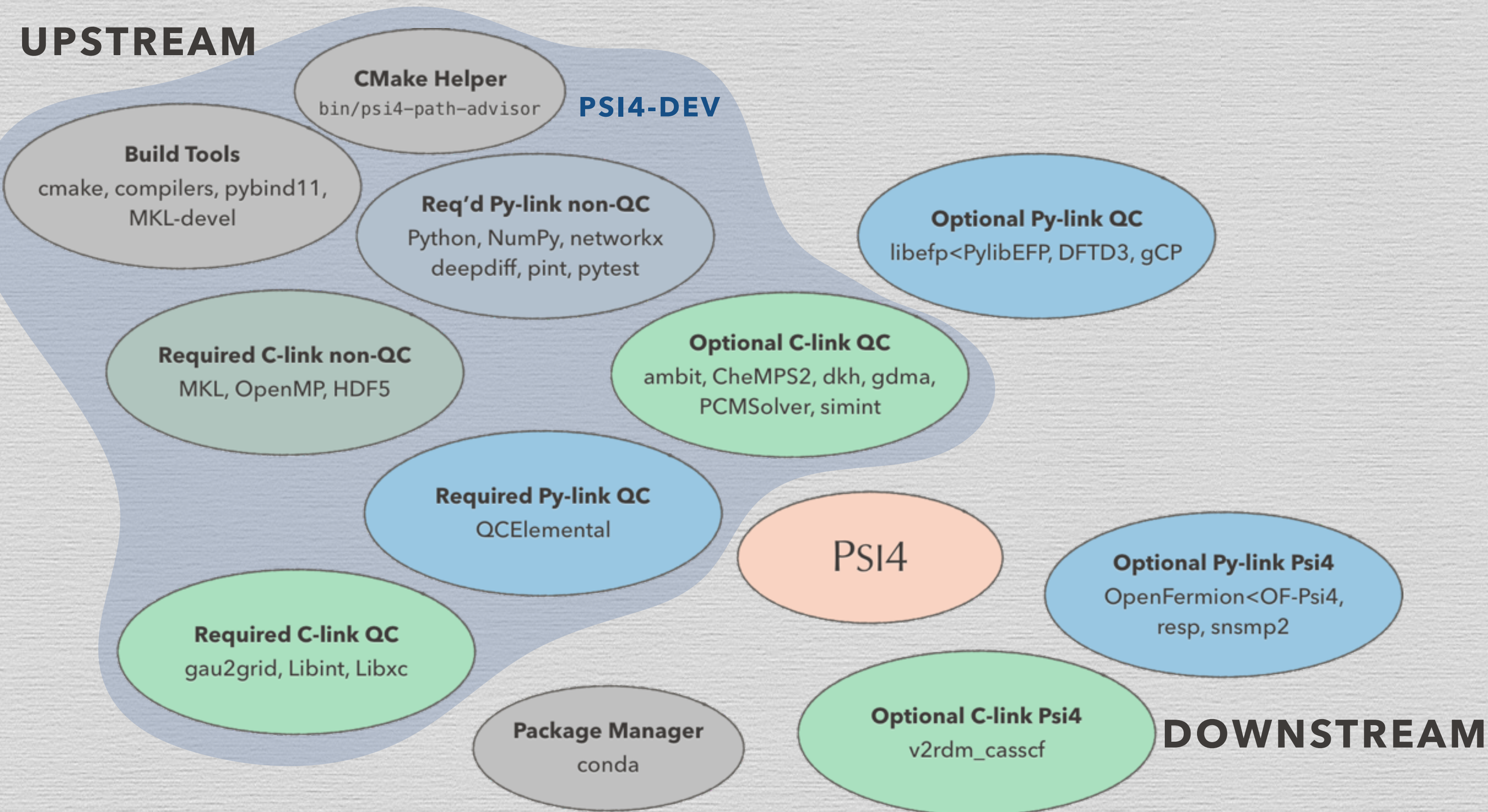


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PSI4 · dependencies · add-ons

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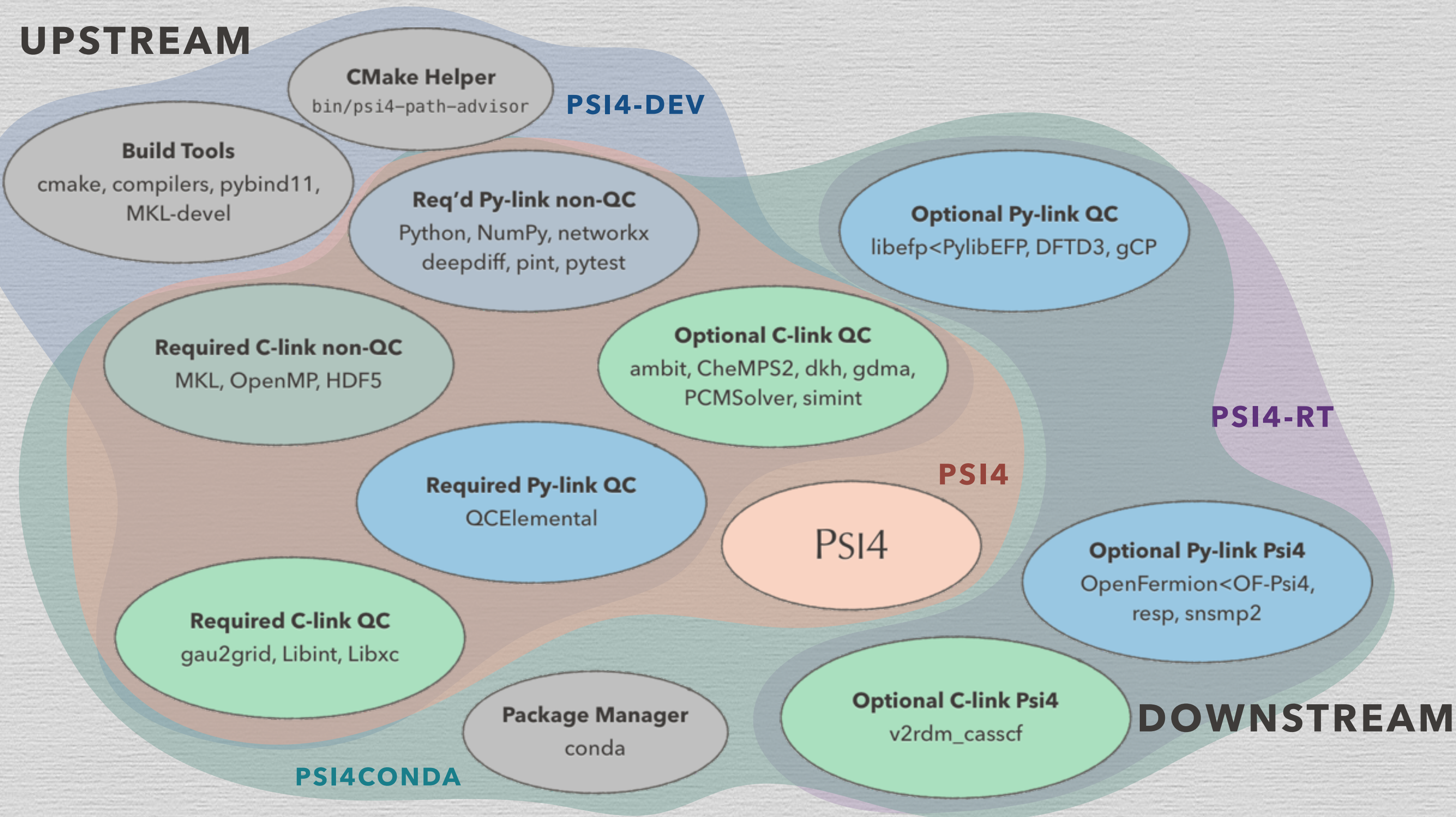
PSI4CONDA



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PSI4 · dependencies · add-ons

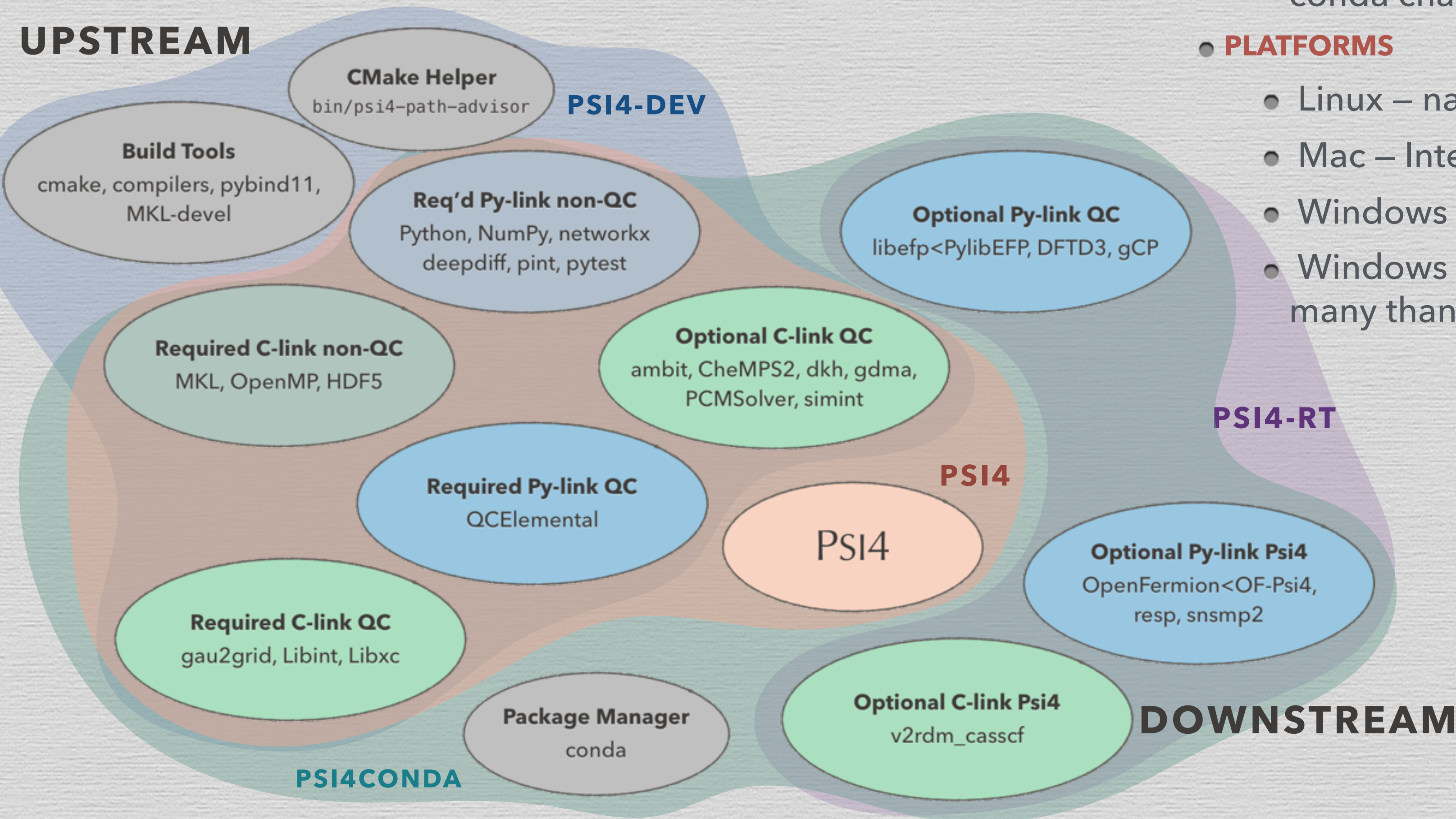
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PSI4 · dependencies · add-ons



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## UPSTREAM



## ● PYTHON

- v3.6 – will be retired soon for packaging but still buildable
- v3.7 – continued support
- v3.8 – continued support
- v3.9 – already buildable; will be packaged when defaults conda channel ready

## ● PLATFORMS

- Linux – naturally
- Mac – Intel processors; no plans yet for new Apple chips
- Windows WSL – uses Linux packages so fully supported
- Windows native – limited ecosystem buildout in progress; many thanks to R. Galvelis & A. C. Simmonett

**CORE DEVELOPERS:**  
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PSi4CONDA