

2018 PSI4 ORDNANCE SURVEY

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9 NOV 2018



UPSTREAM

BLAS-LAPACK
FORTRAN LIBRARY
BSD-3-Clause

optking
PYTHON LIBRARY
BSD-3-Clause

Libint
C LIBRARY
LGPL-3.0+

PSI3
C++ EXECUTABLE
GPL-2.0

PSI3

DEP is req'd RT
dep'd'cy of TGT

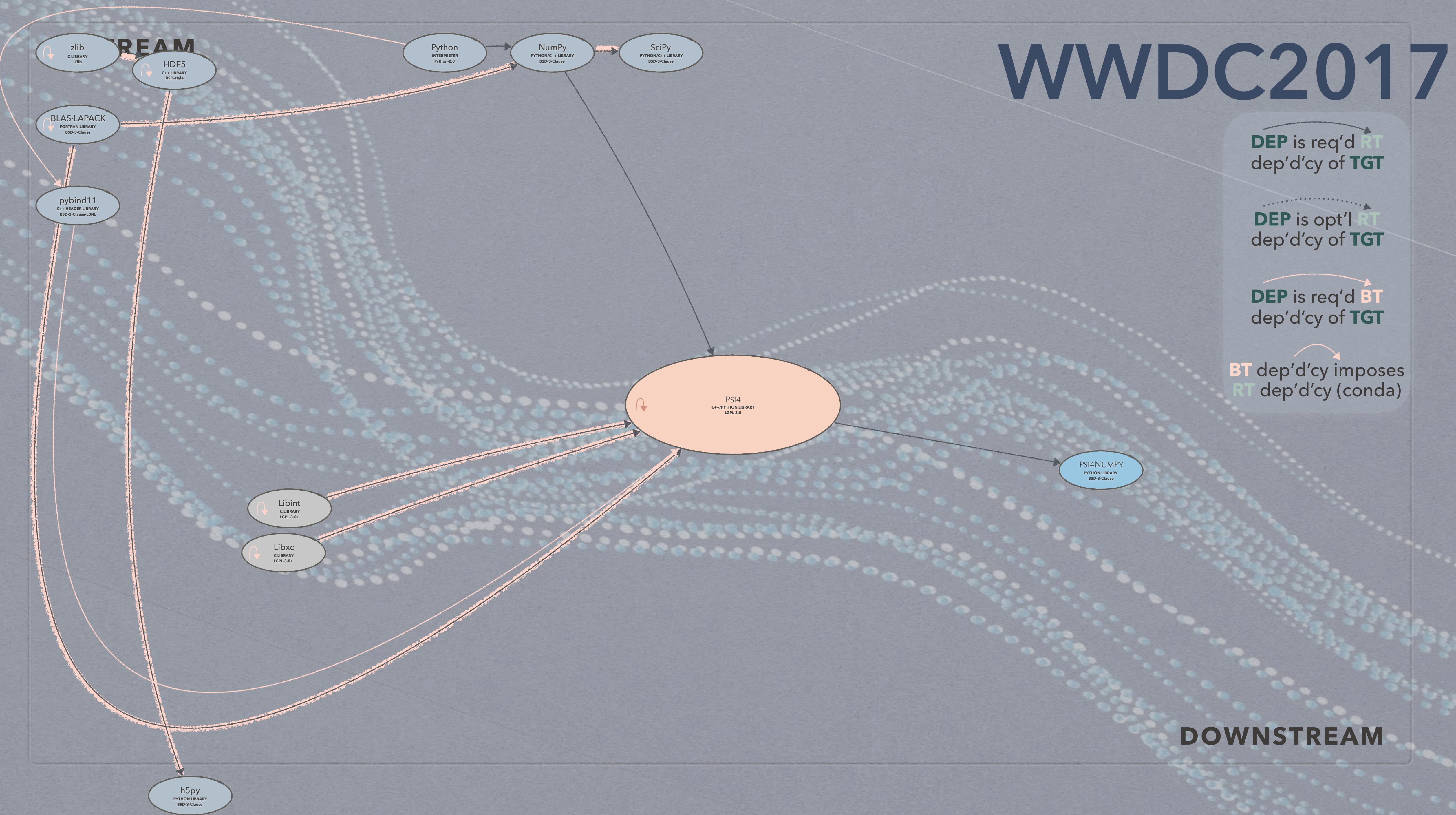
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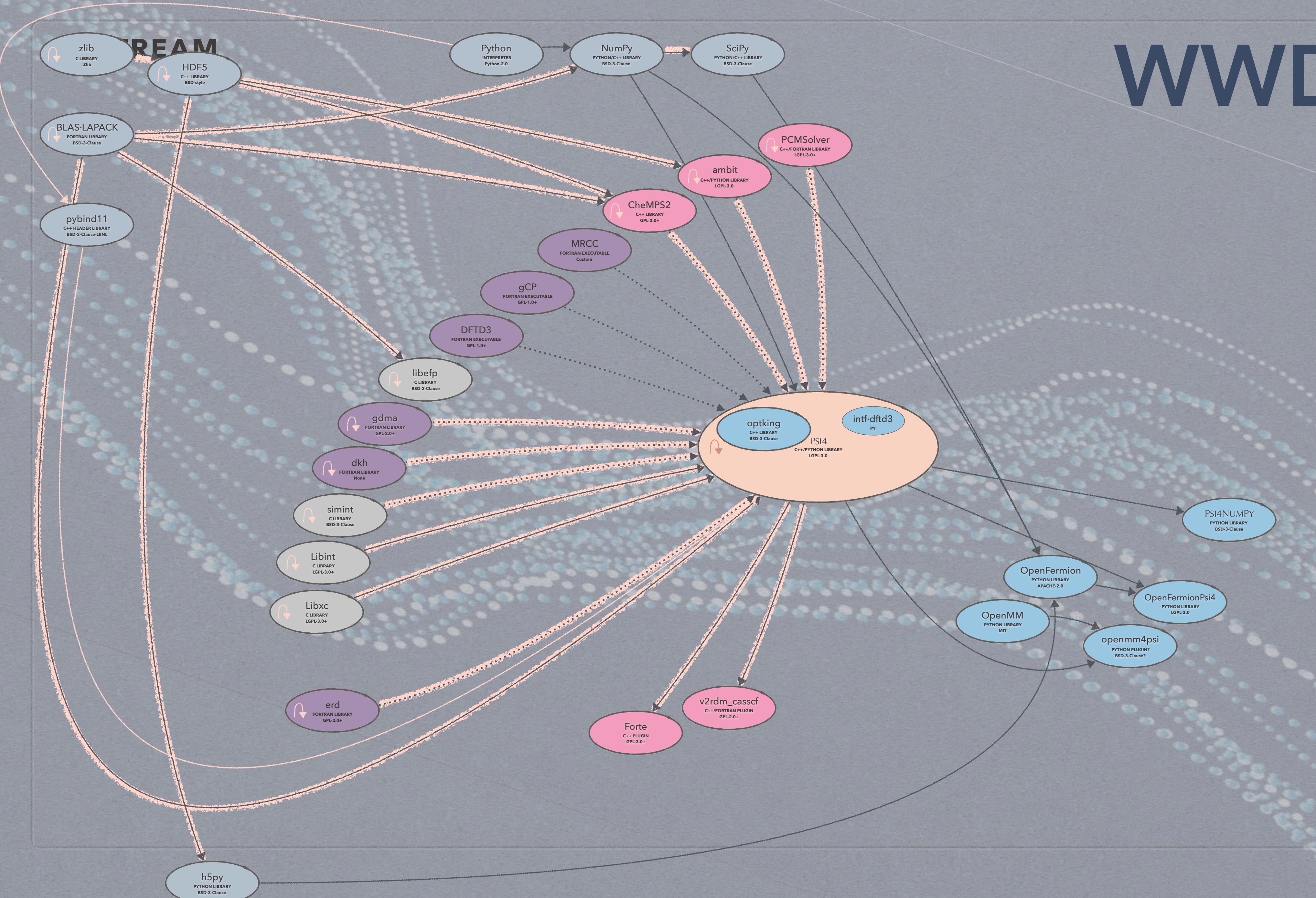
BT dep'd'cy imposes
RT dep'd'cy (conda)

DOWNSTREAM

WWDC2017



WWDC2017



Themes

- disgorging others' projects from codebase
- facilitating downstream w/ plugins
- augmenting capabilities w/ others' projects

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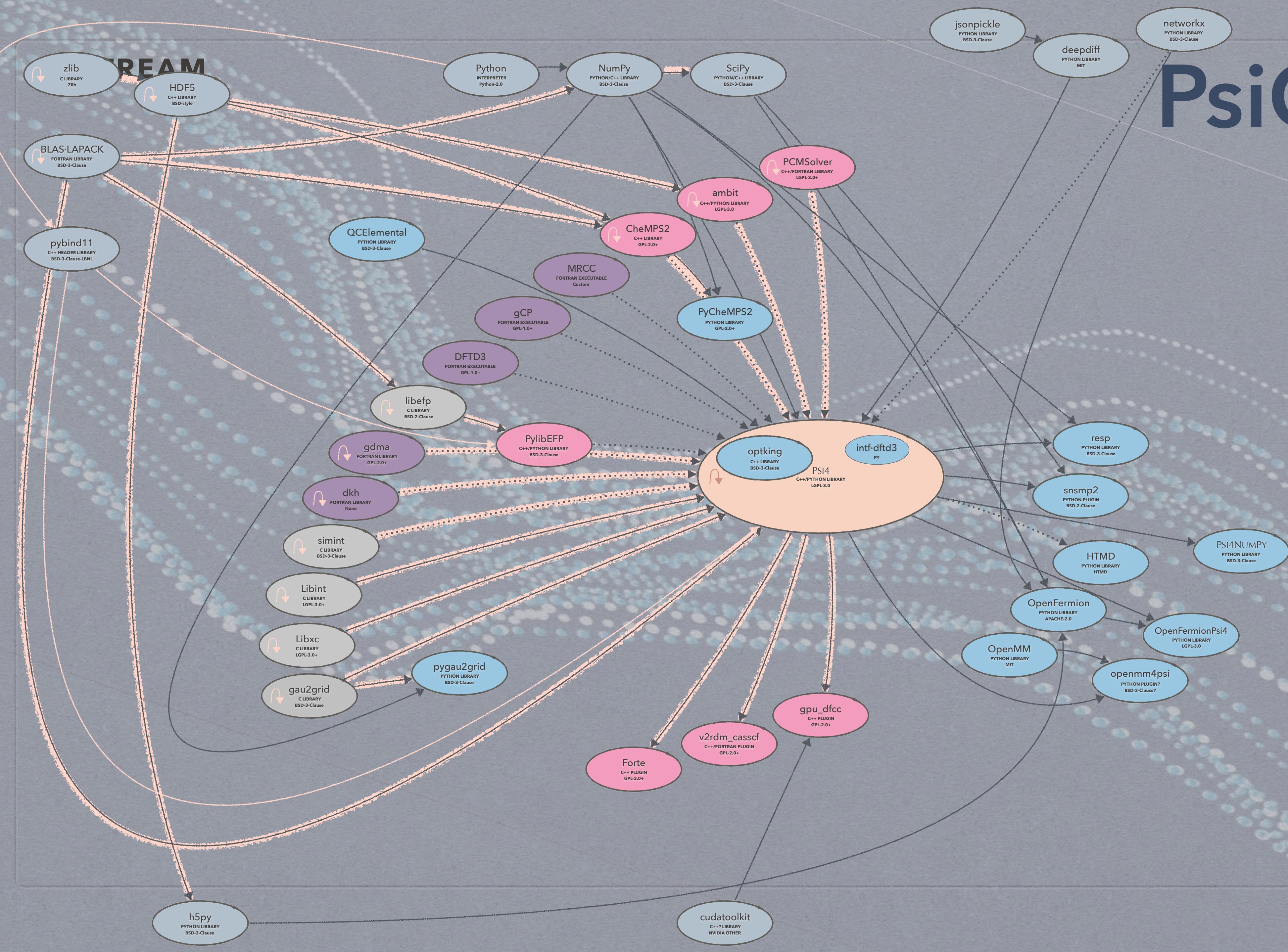
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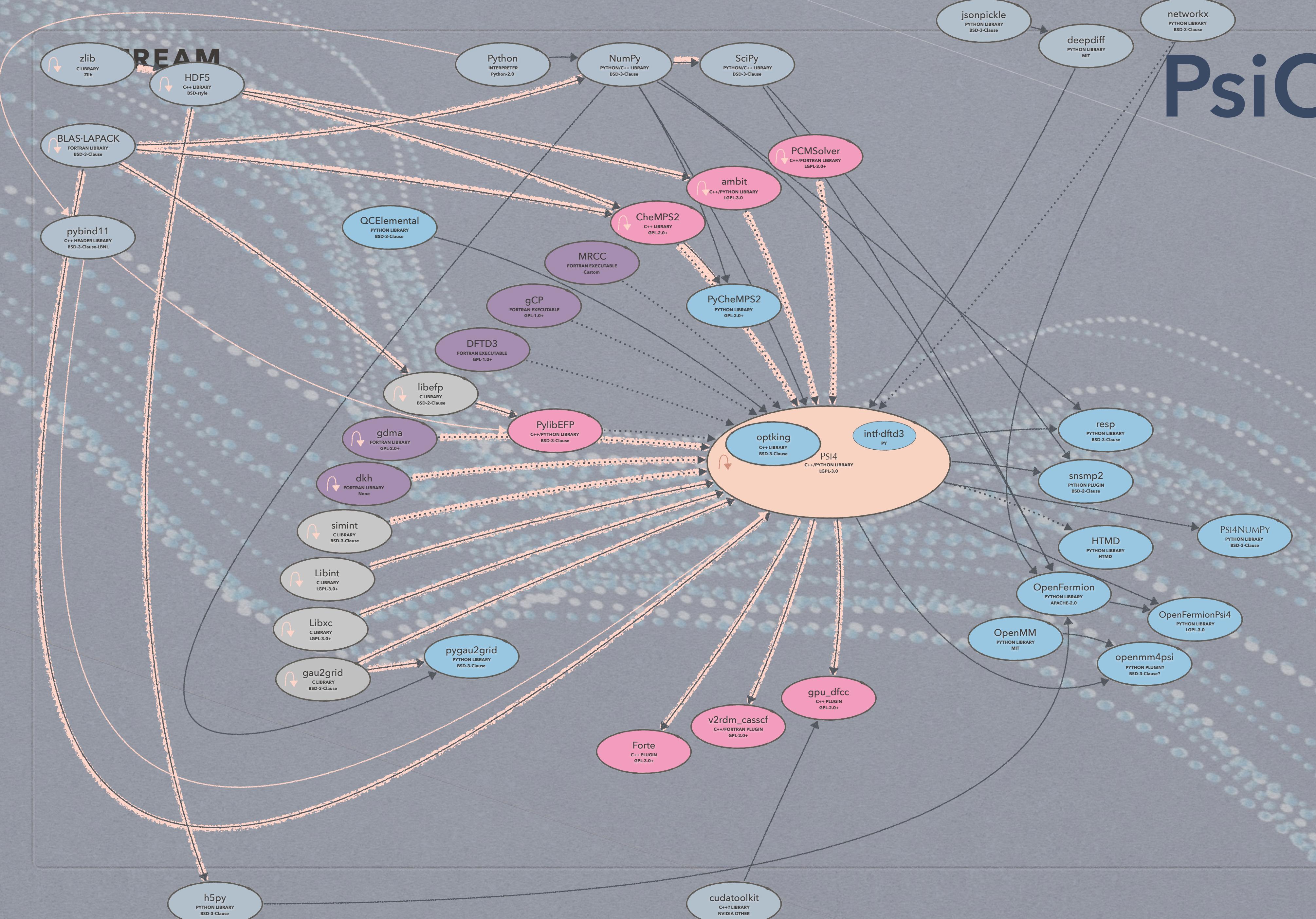
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gau2grid

- Daniel Smith's library for gaussians on a grid
- replaces Psi4 code and makes DFT faster

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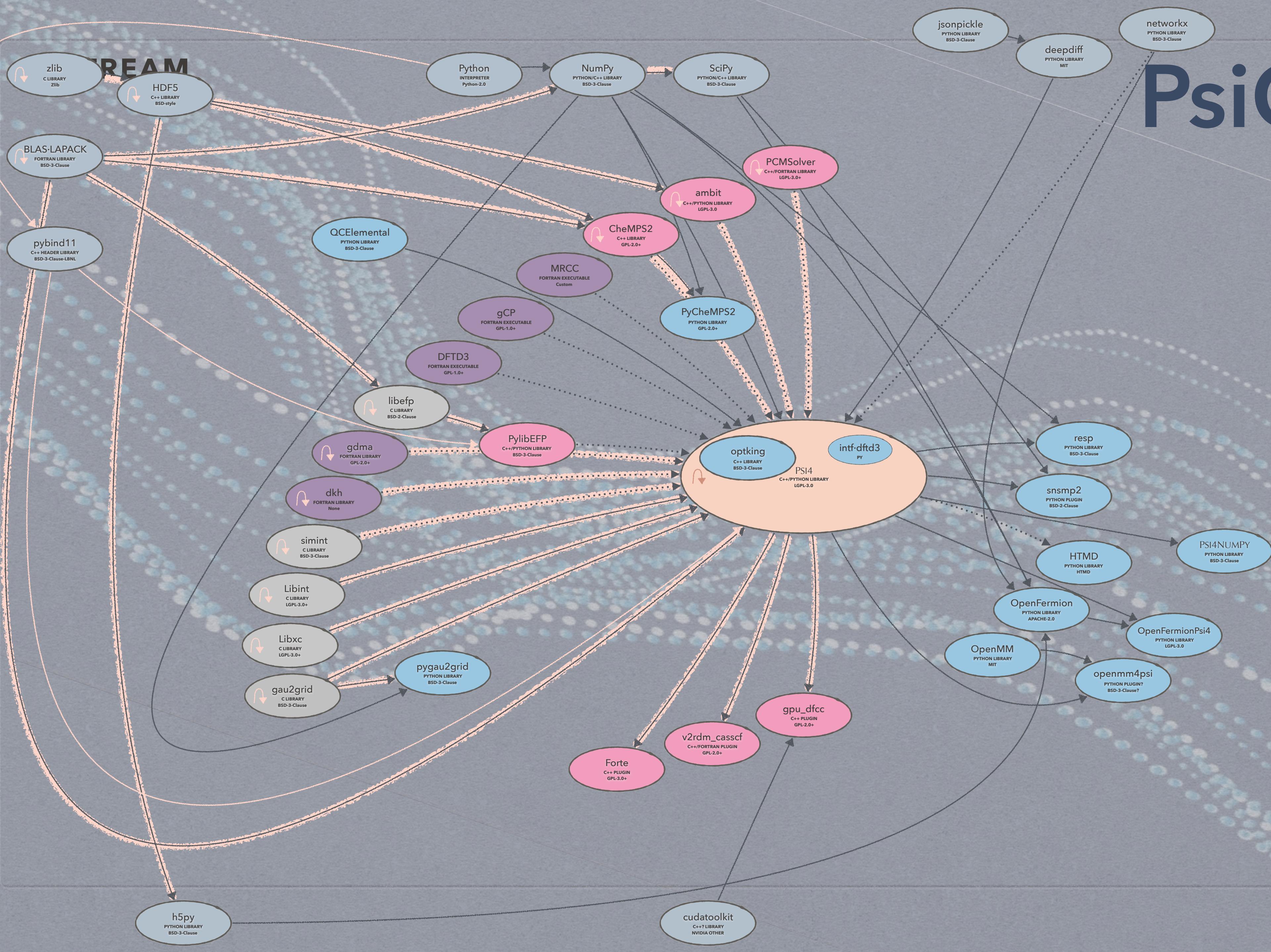
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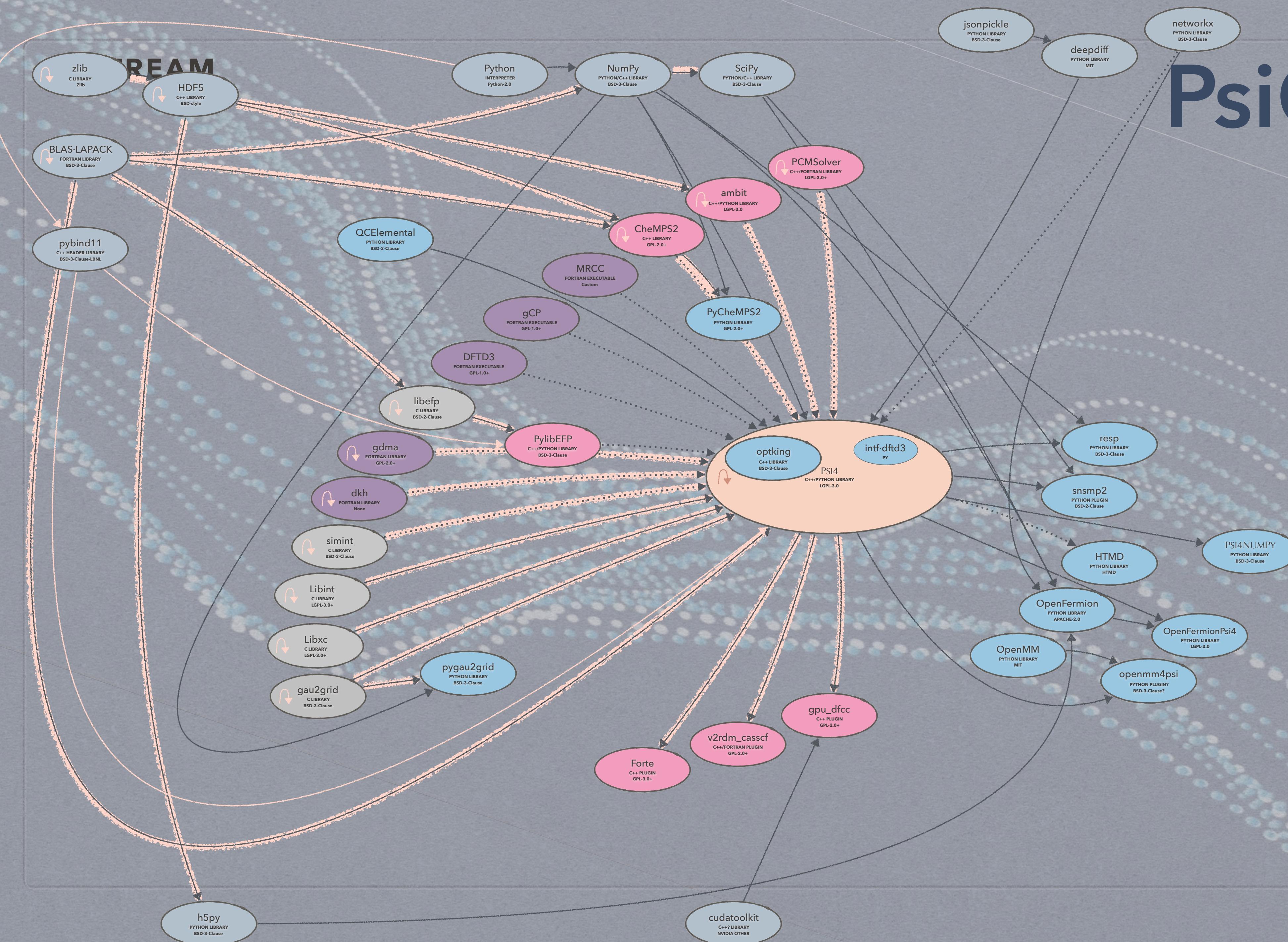
pybind11

- v2.0 → v2.2
- now safe to mix pb11 project
- the cost is PSI_API

DOWNSTREAM



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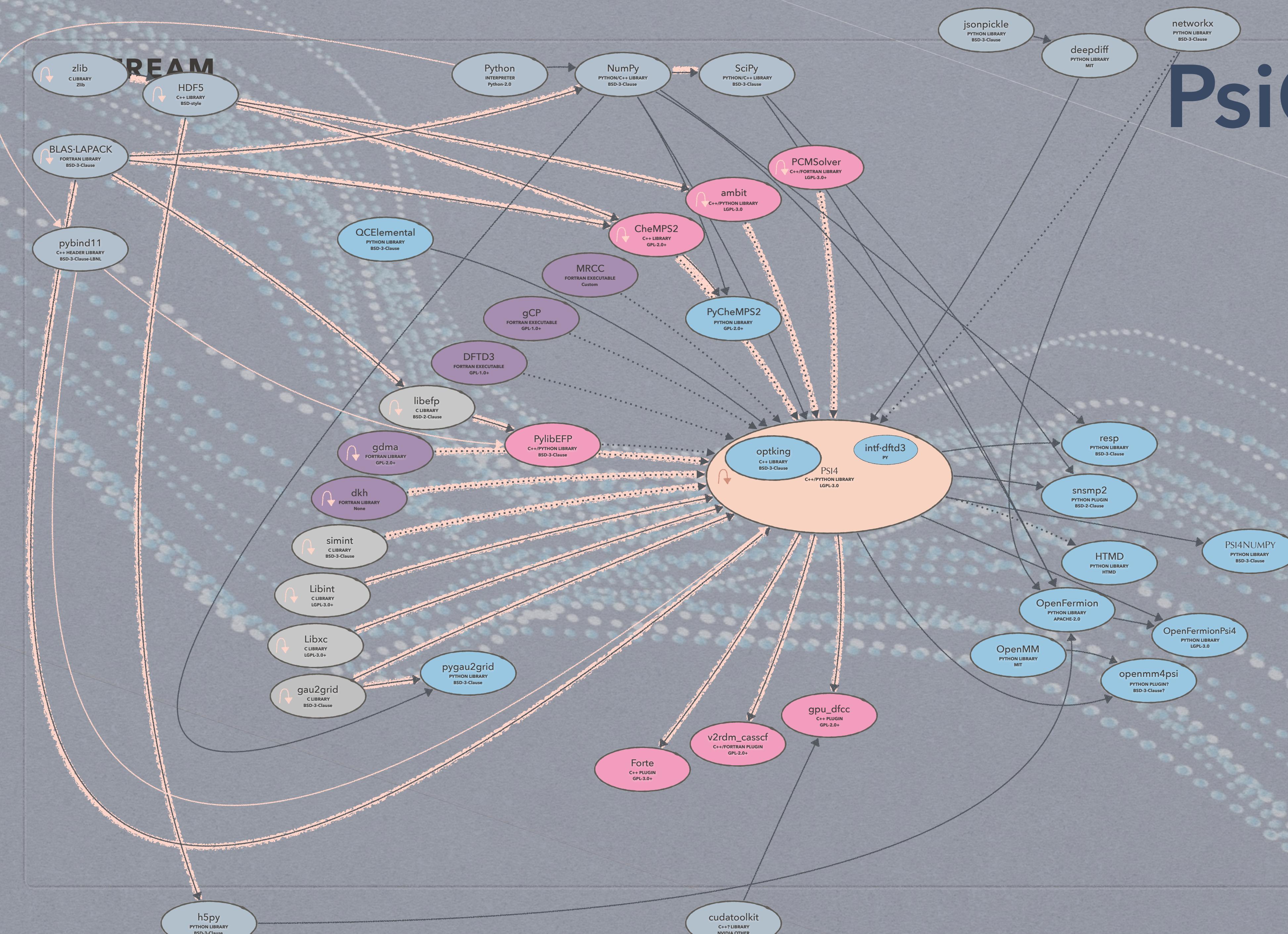
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Libint

- primary integrals library
- only integrals lib we use for deriv
- Strategy Q?: distribute AM8 on Linux at cost of fatter package?

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Libxc

- density functional library
- using v3 fork. could alternately use v4 fork
- communication difficulties moving to upstream

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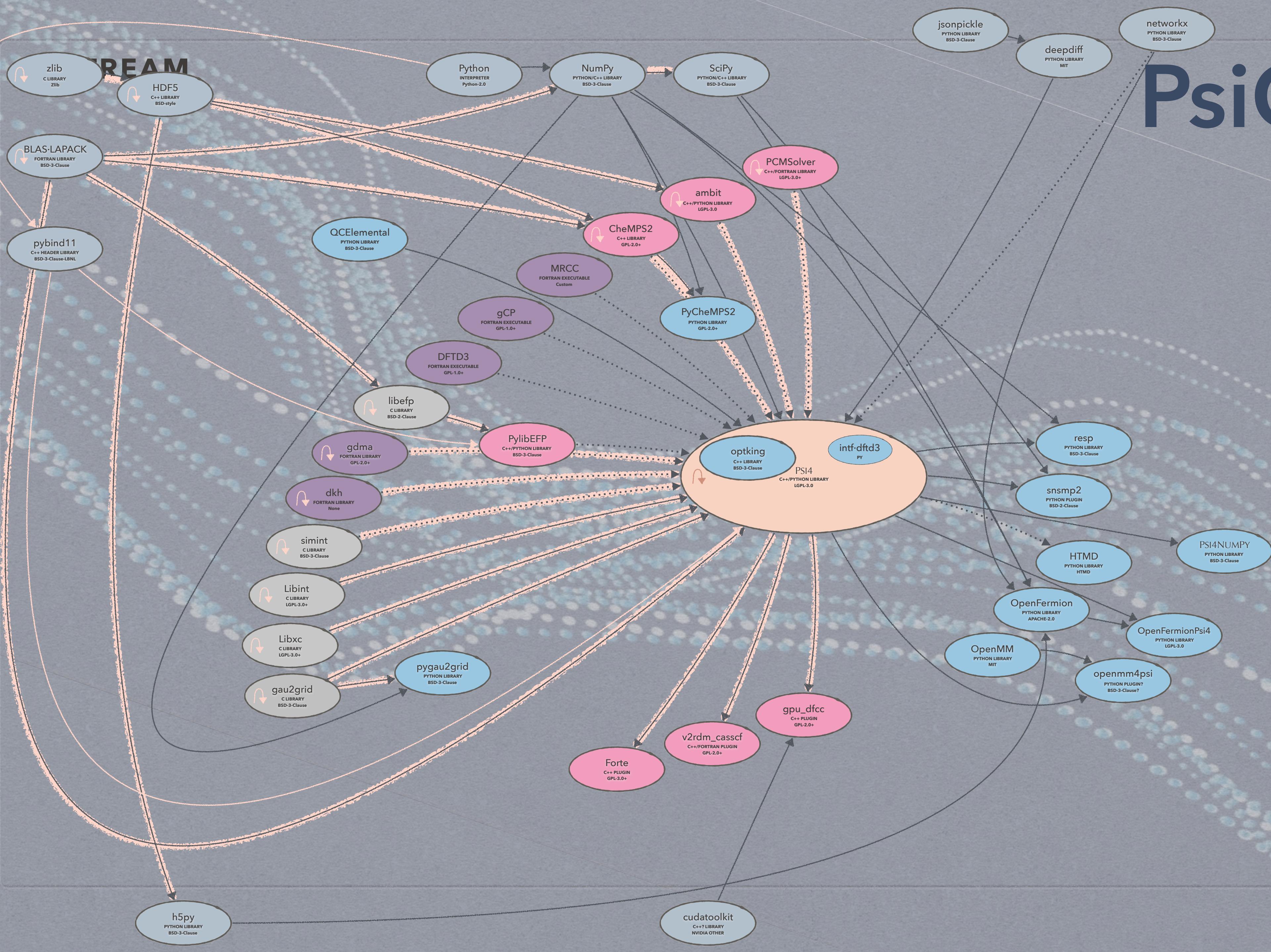
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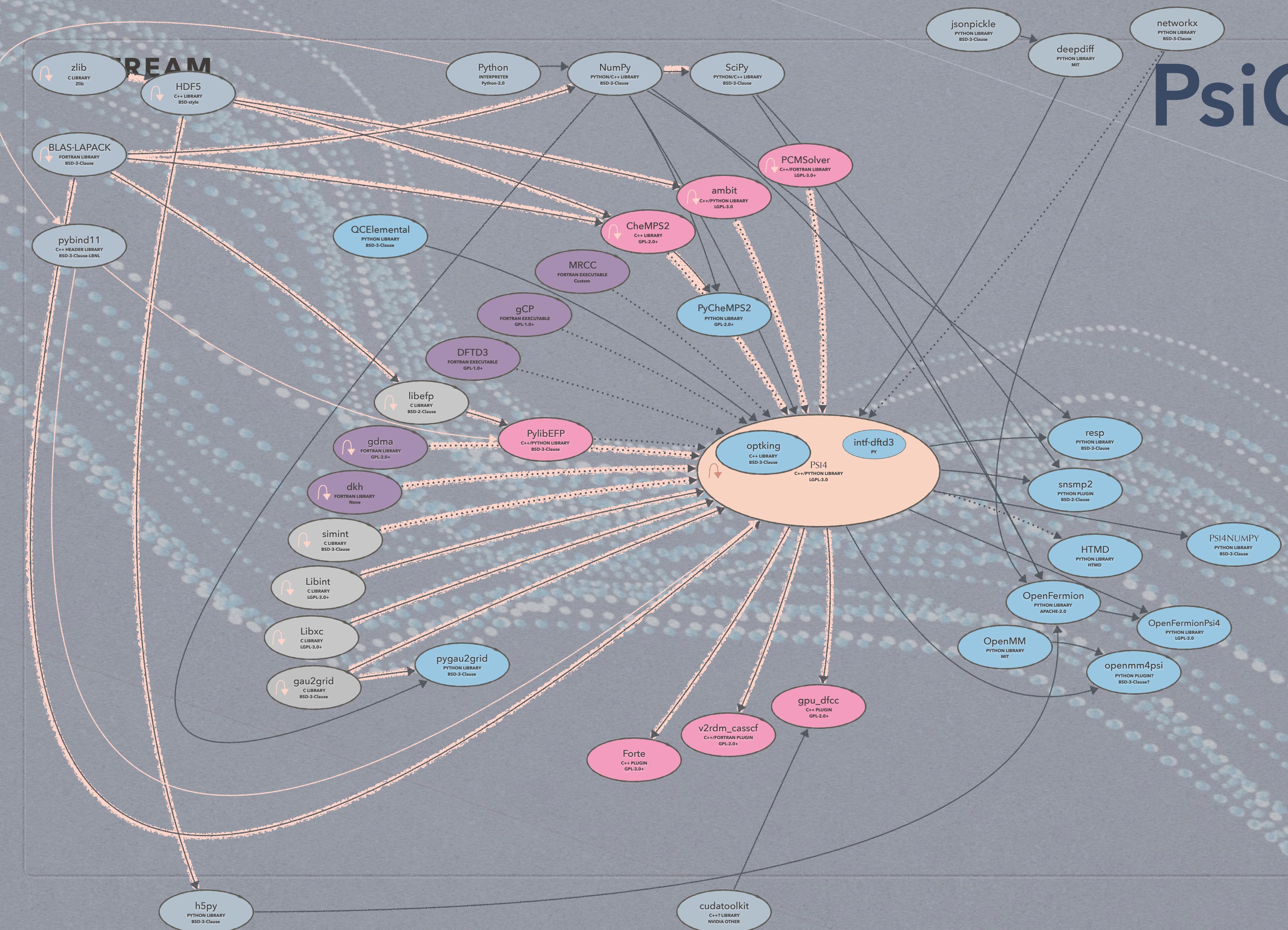
ERD

- lost – interface broken
- no research interest in fixing it

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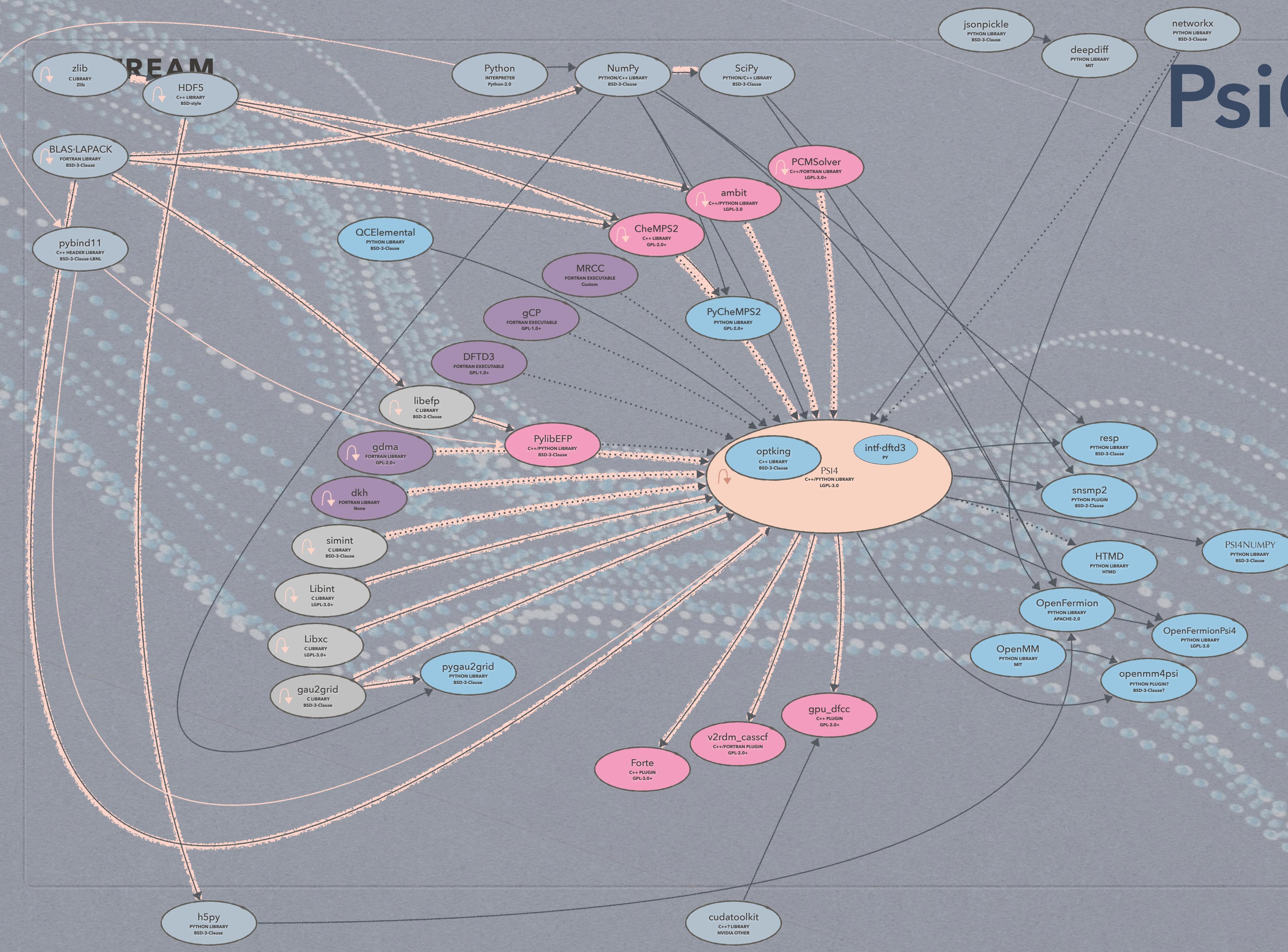


Simint

- alternate integrals library for plain ints
- deriv ints available but not interfaced
- storage in libmints would need revamping to take full adv of vectorization

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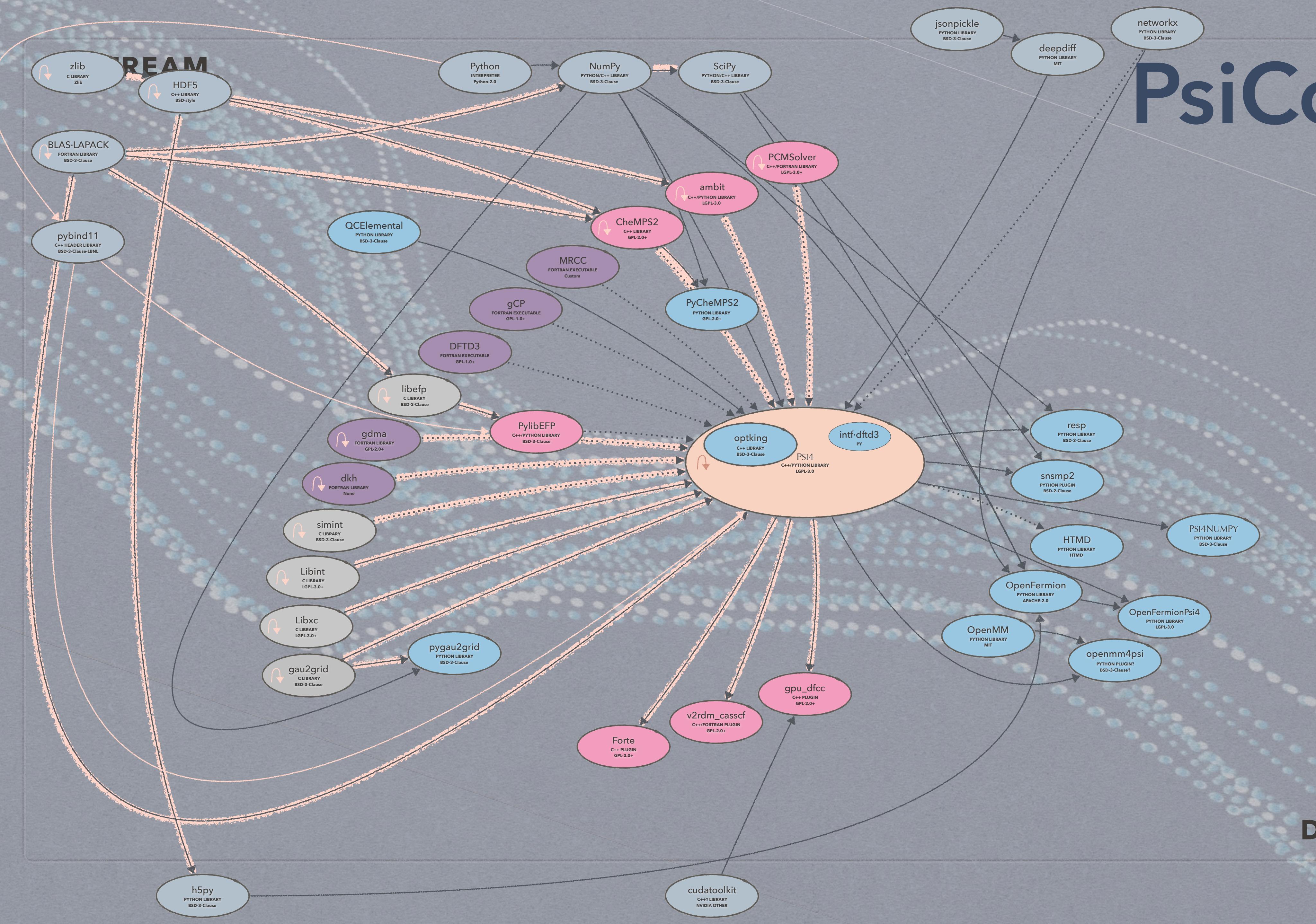
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EFP

- EFP octopus dis-armed
- call PylibEFP for EFP/EFP and in py-side SCF/EFP

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QCElemental

- CODATA 2014): c-side header, py-side API call
- periodic table: c-side header (~unused), py-side API call; fixed mass errors
- molecule parsing & schema gen

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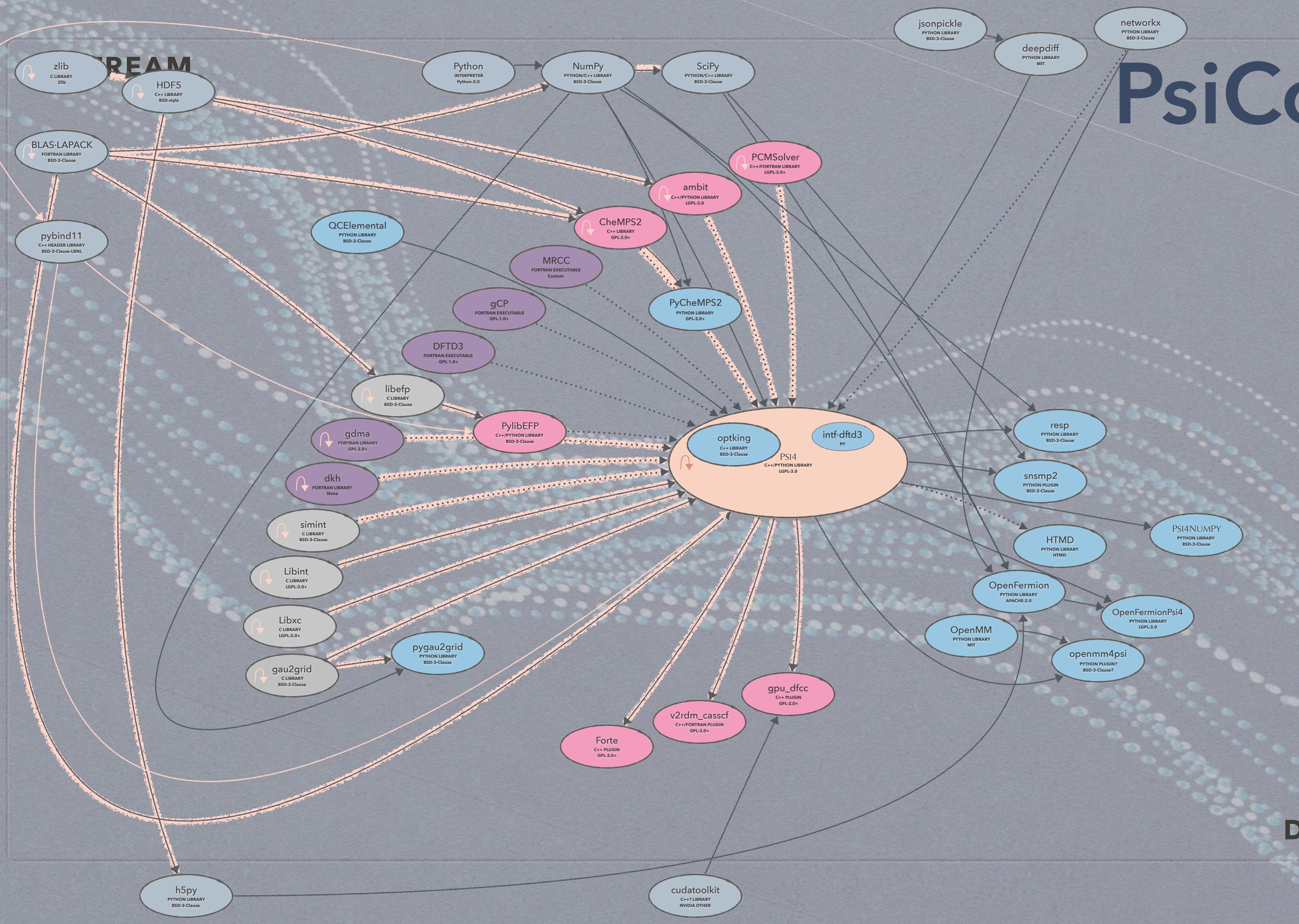
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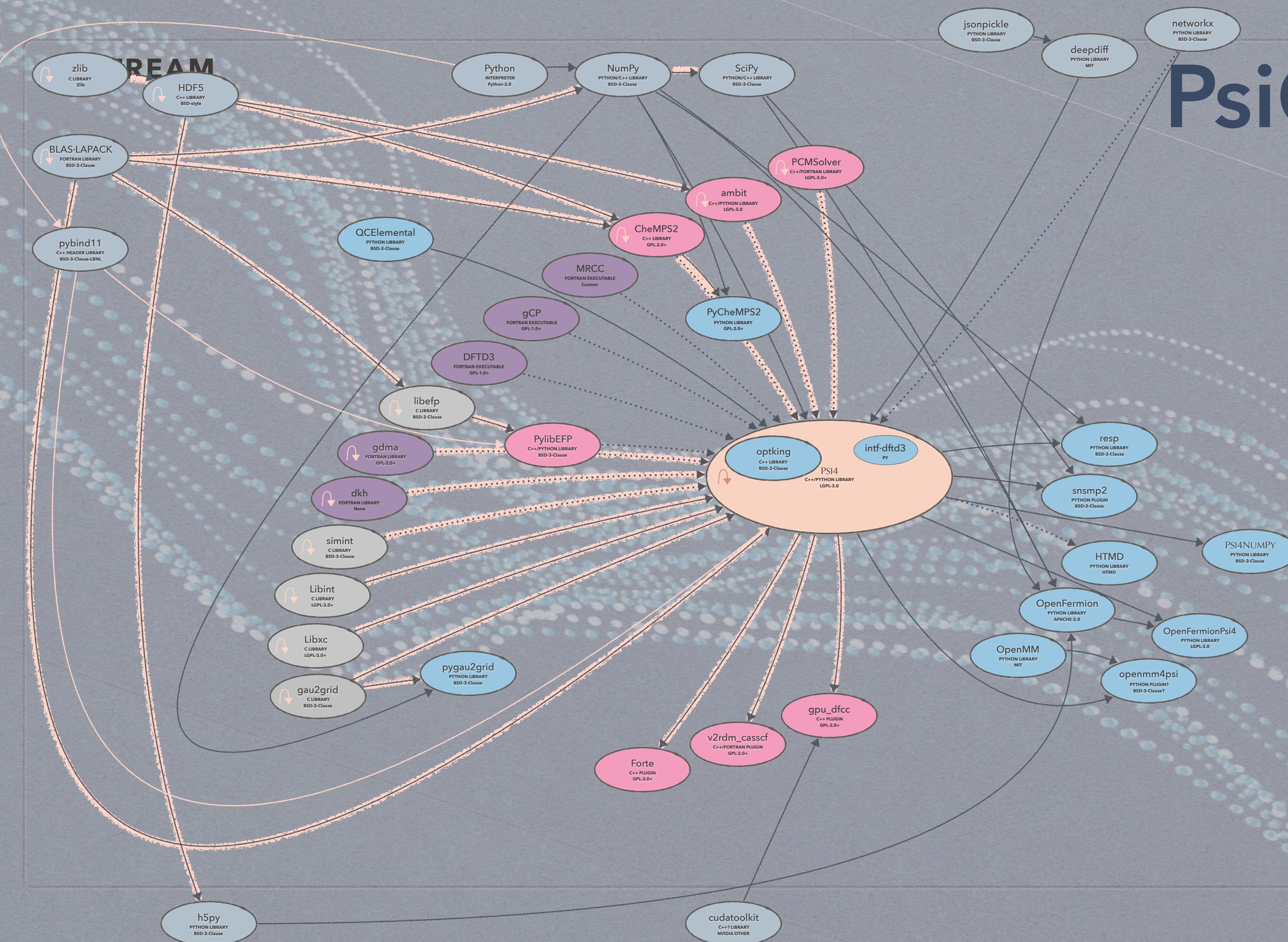
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snsmp2

- Robert McGibbon/DE Shaw pure-py plugin
- snsmp2 energy method



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resp

- Asim Alenaizan pure-py plugin
- RESP charges from Psi or GAMESS

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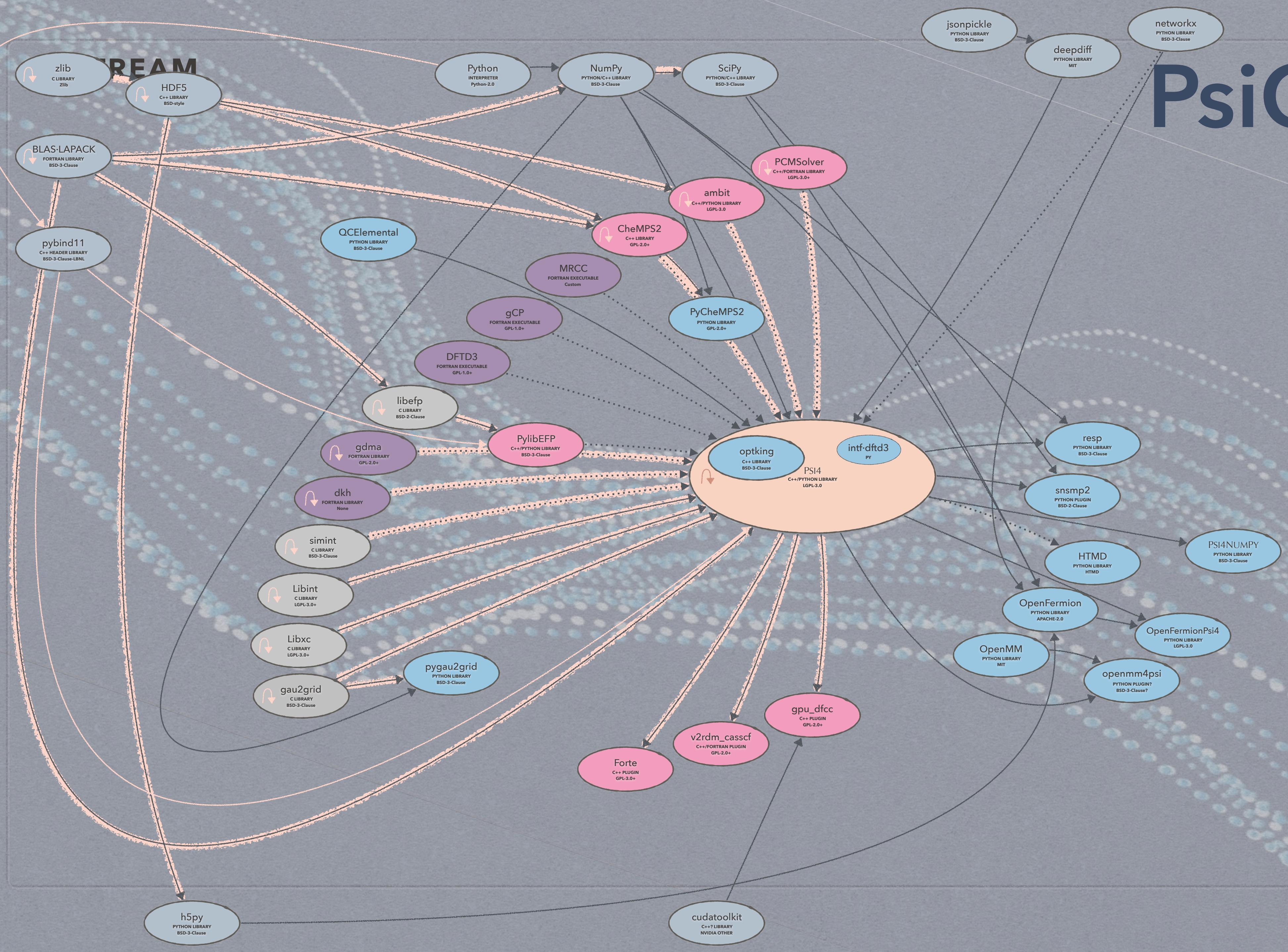
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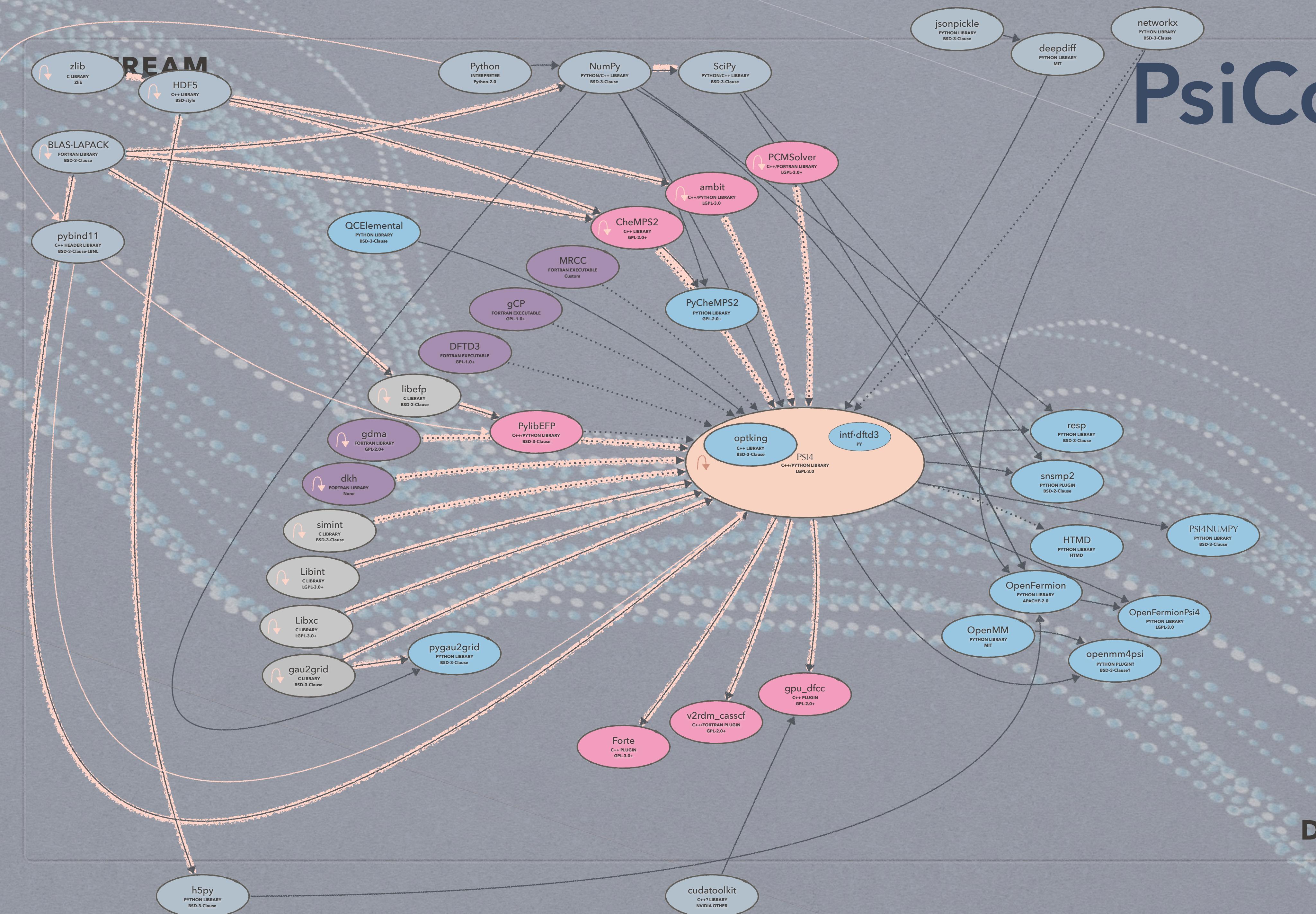
gpu_dfcc

- Eugene DePrince III compiled plugin
- GPU coupled cluster
- all software avail on conda bring your own hardware

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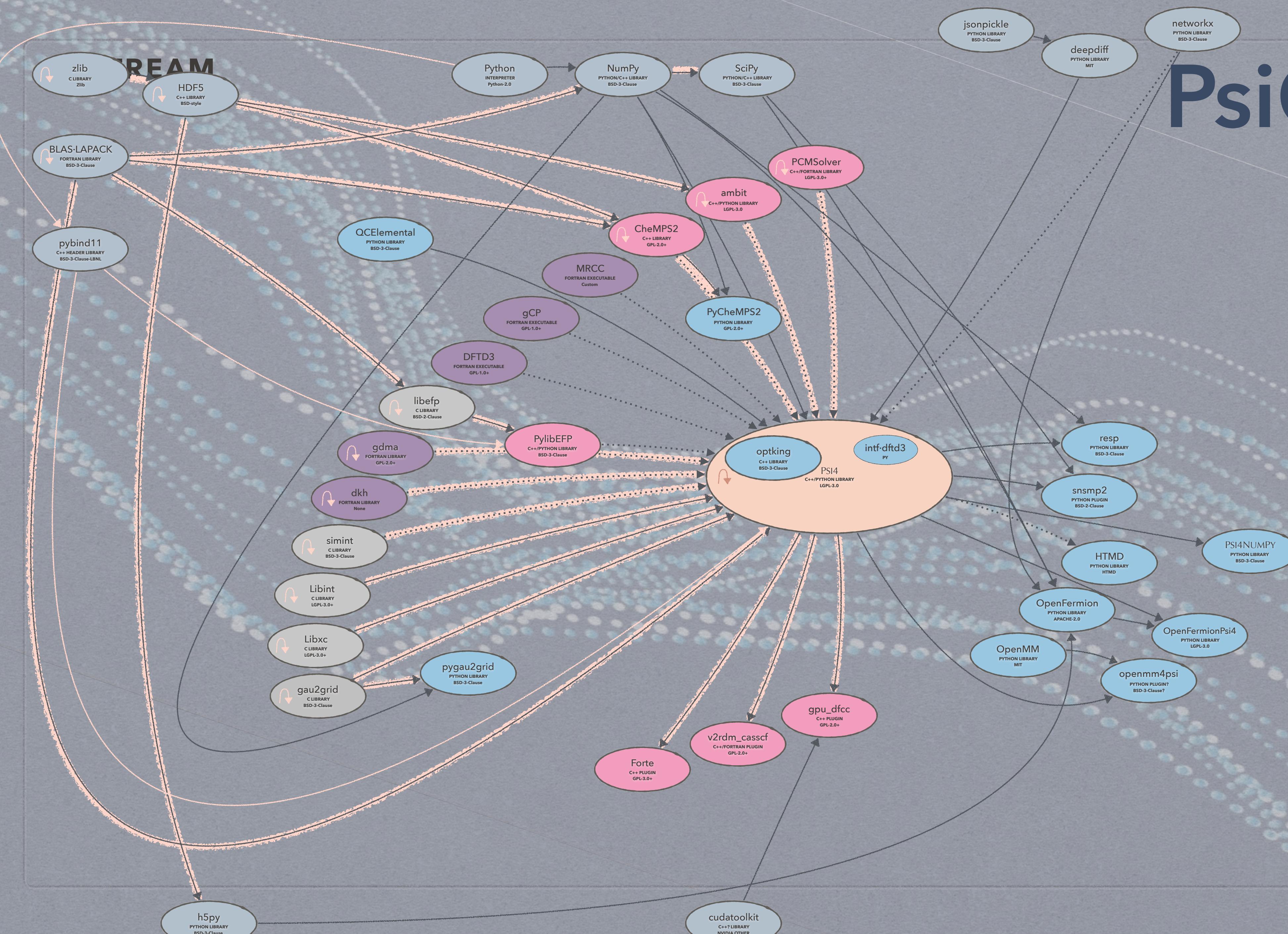
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HTMD

- Acellera using Psi Folding@home-like environment
- handsome donation of Windows porting
- running on limited hardware – good if Psi could adapt

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Themes

- working to use up/downstream, not forks
- growing plugin collection; ABI changes aggravate
- refactoring dependencies

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Future

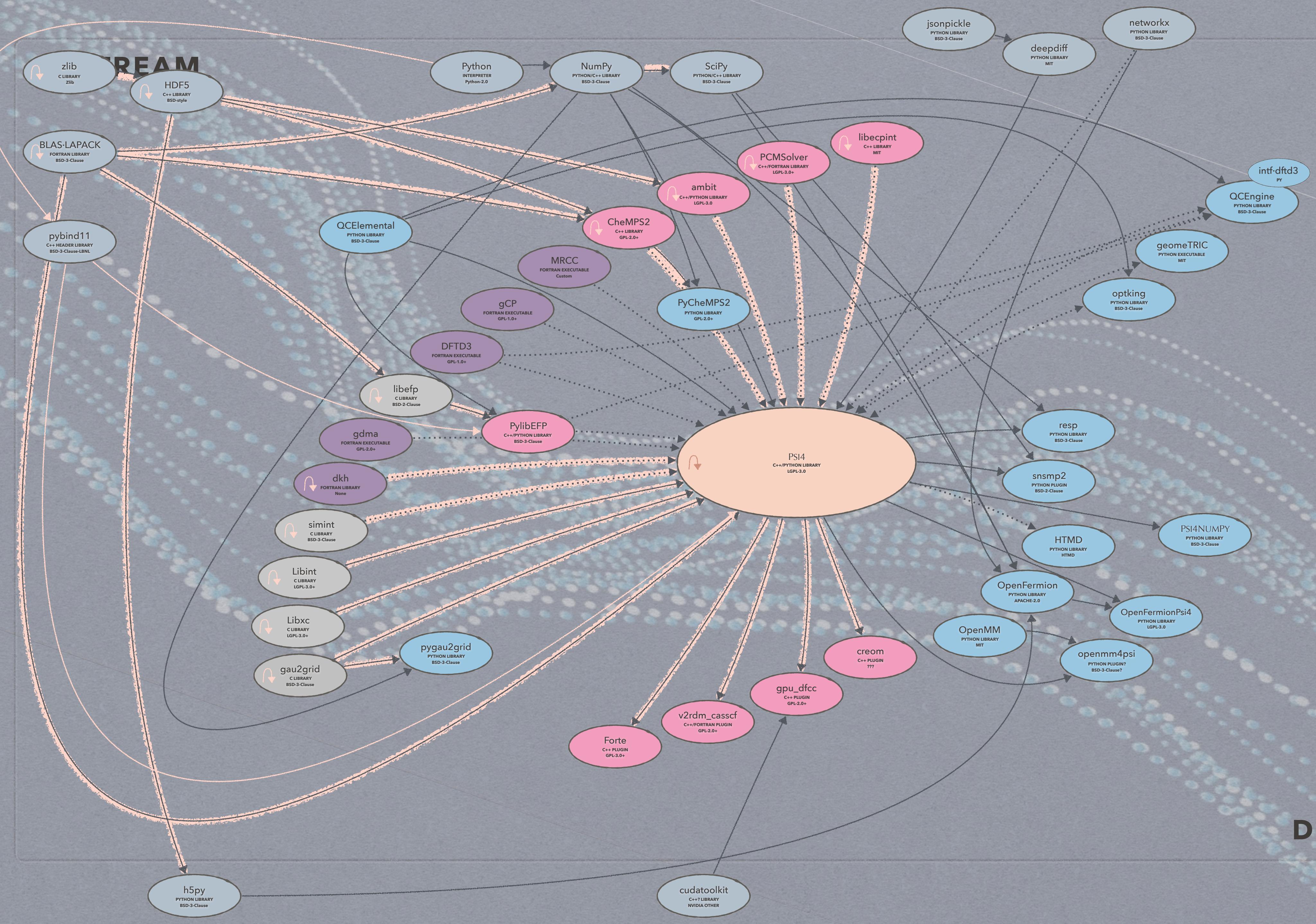
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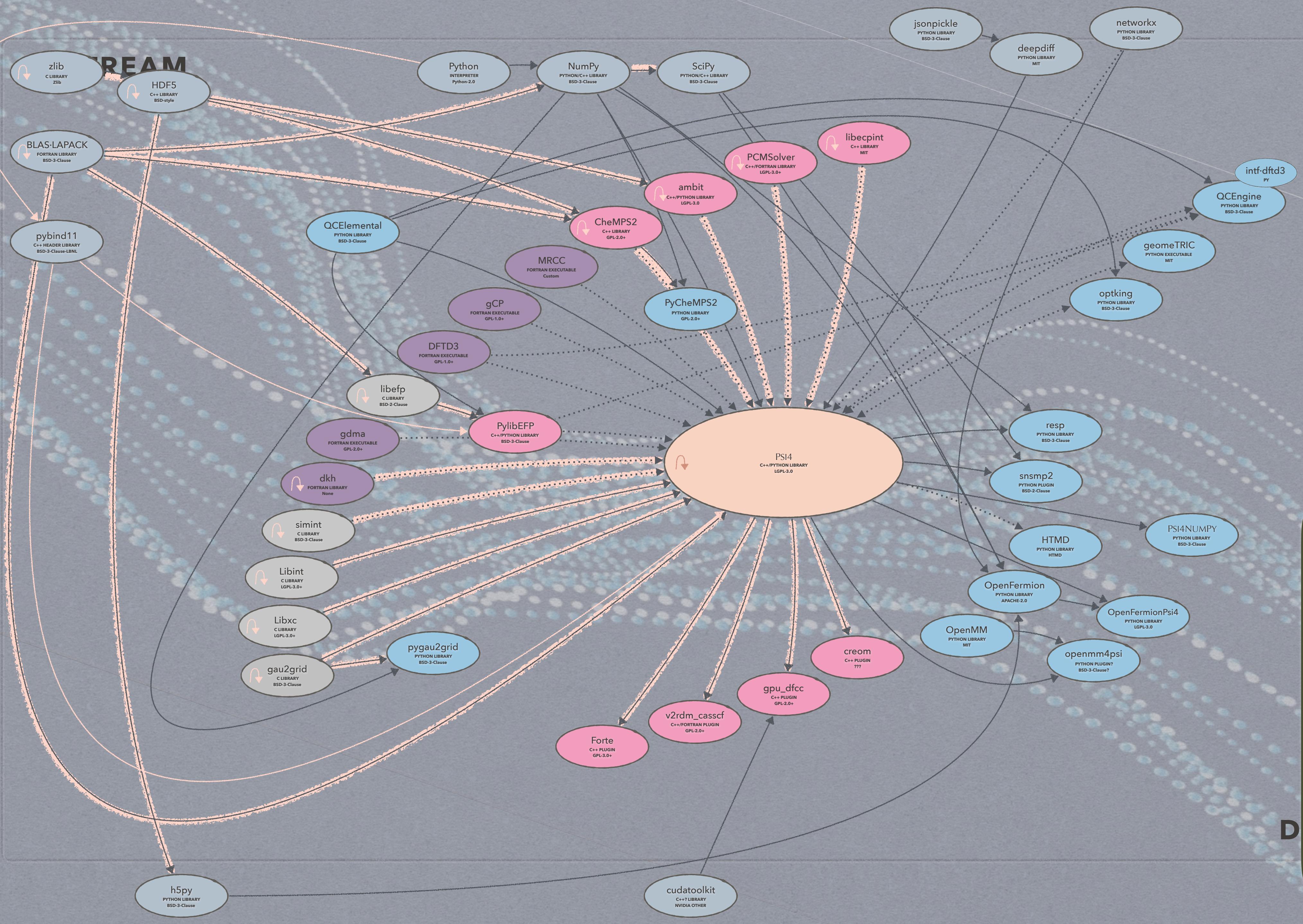
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GDMA

- no current reason it should be a library, not wrapped exe
- I want to switch to exe for (1) no fork, (2) updates, (3) reuseability

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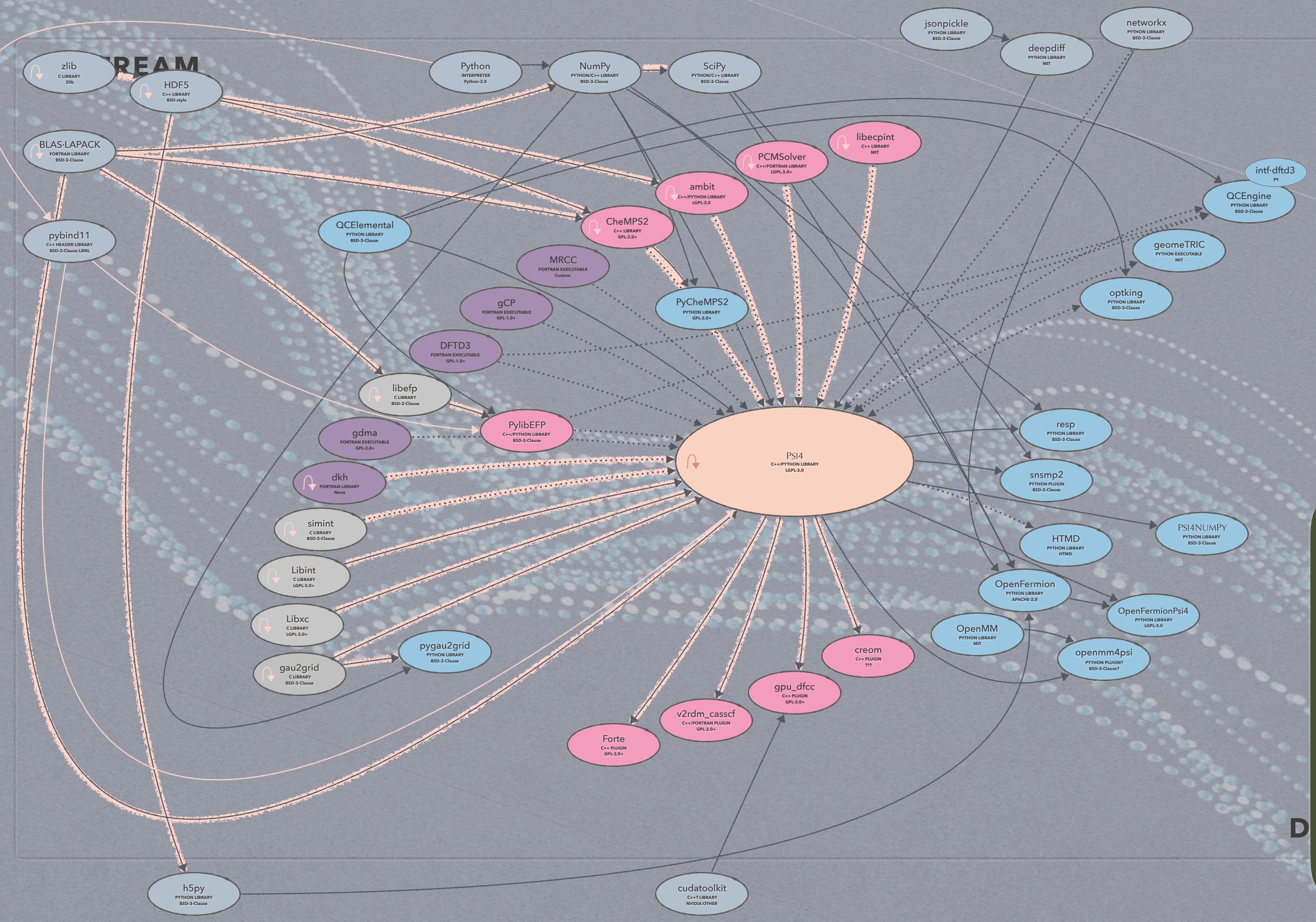
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QCEngine

- takes QCSCHEMA, returns QCSCHEMA
- rather than API calling some of our light deps, I want to ngl call EFP/EFP, DFTD3
- our interfaces become others' reuseable comp.



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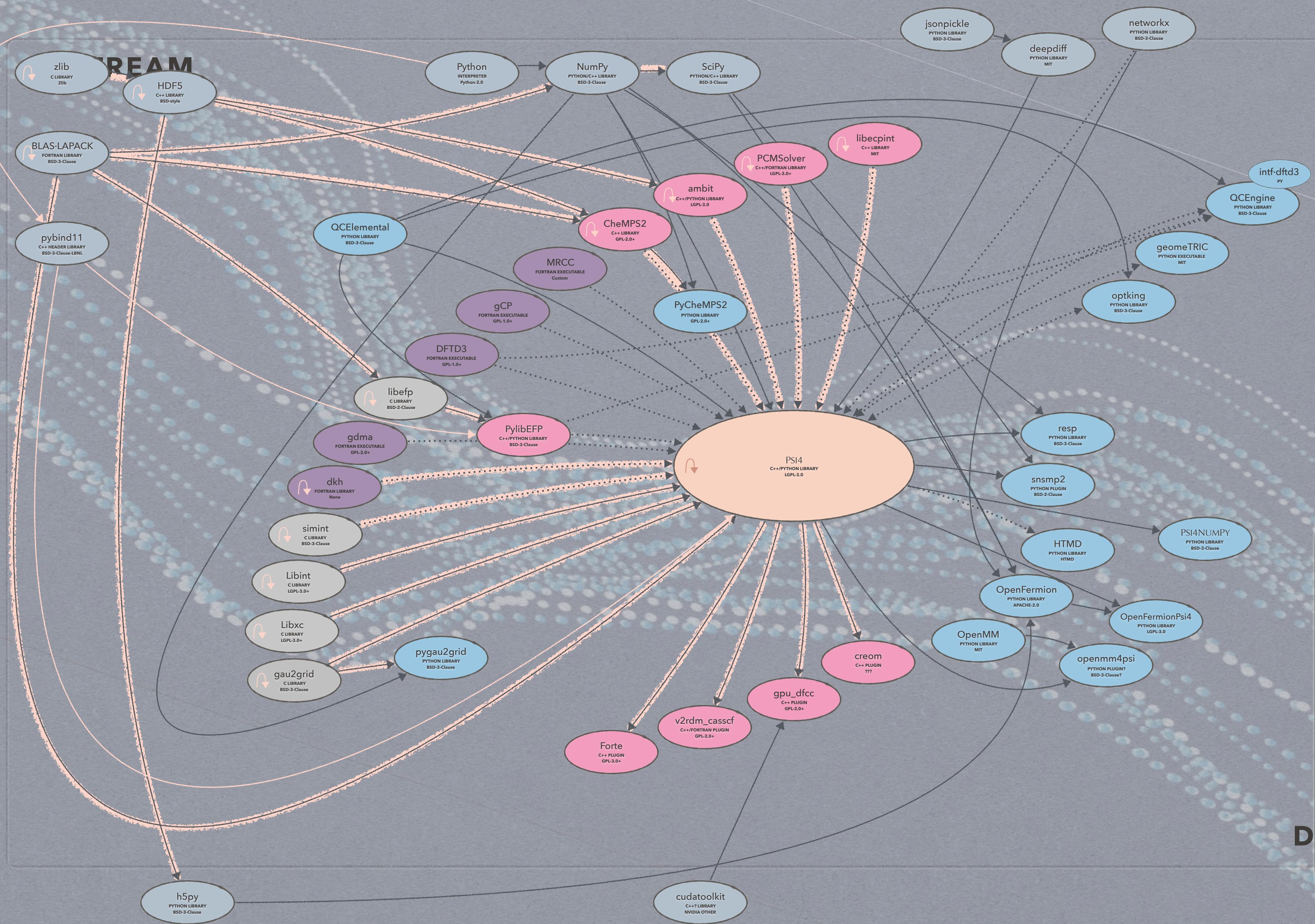
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CheMPS2

- Strategy Q?
replace with PyChemPS2
- easier interface
worth losing C++
API and ||ism?



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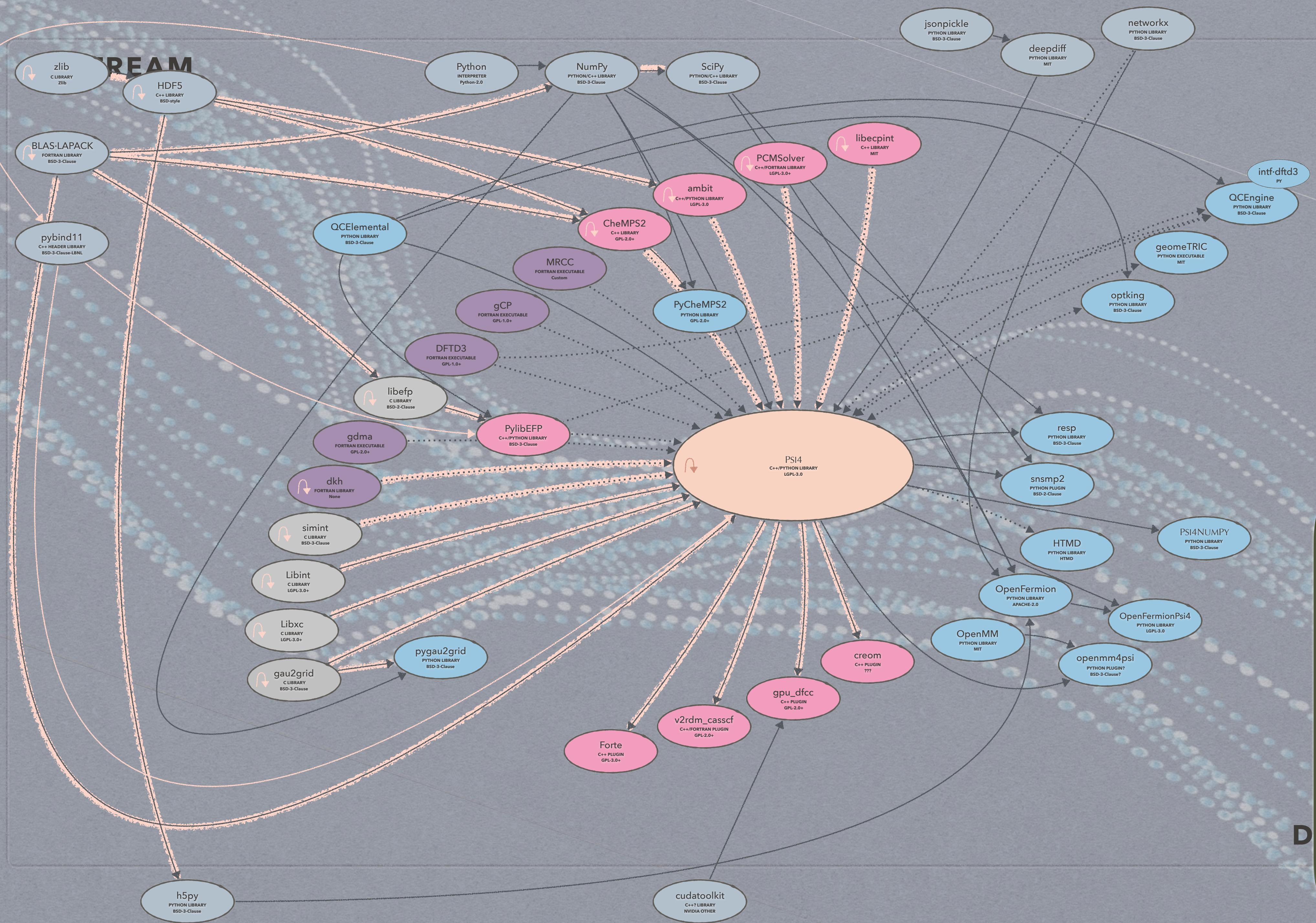
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ECP

- Robert Shaw's indep lib, research sucessor to ECP code currently in Psi
- switch libcpint
- hopefully go faster
- smart SCF prob. needed, too

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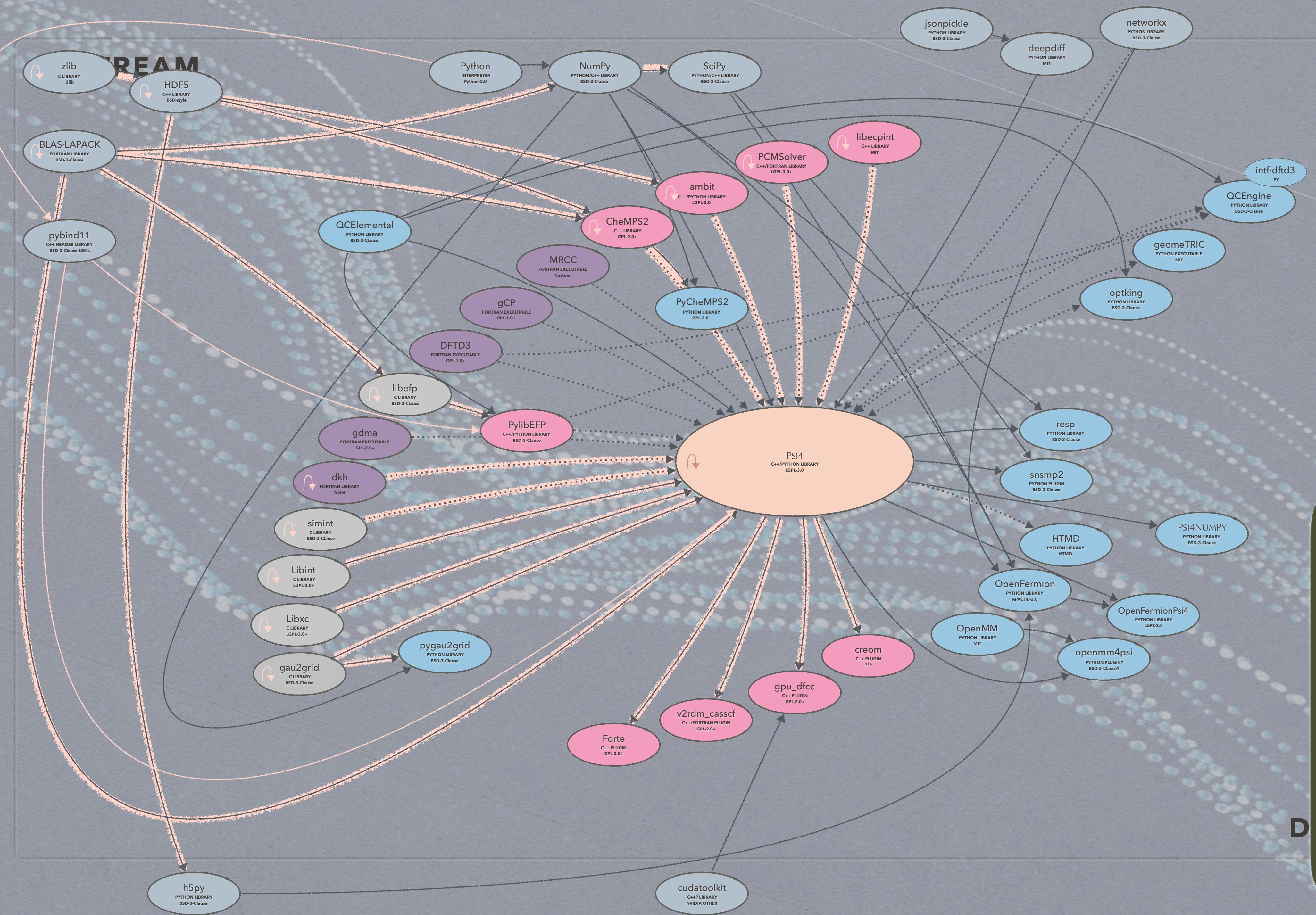
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Optimize

- py-optking mostly working
- need final push before fully capable + merge
- then replace its intf w/field-tested geomeTRIC intf
- then add geomeTRIC, too



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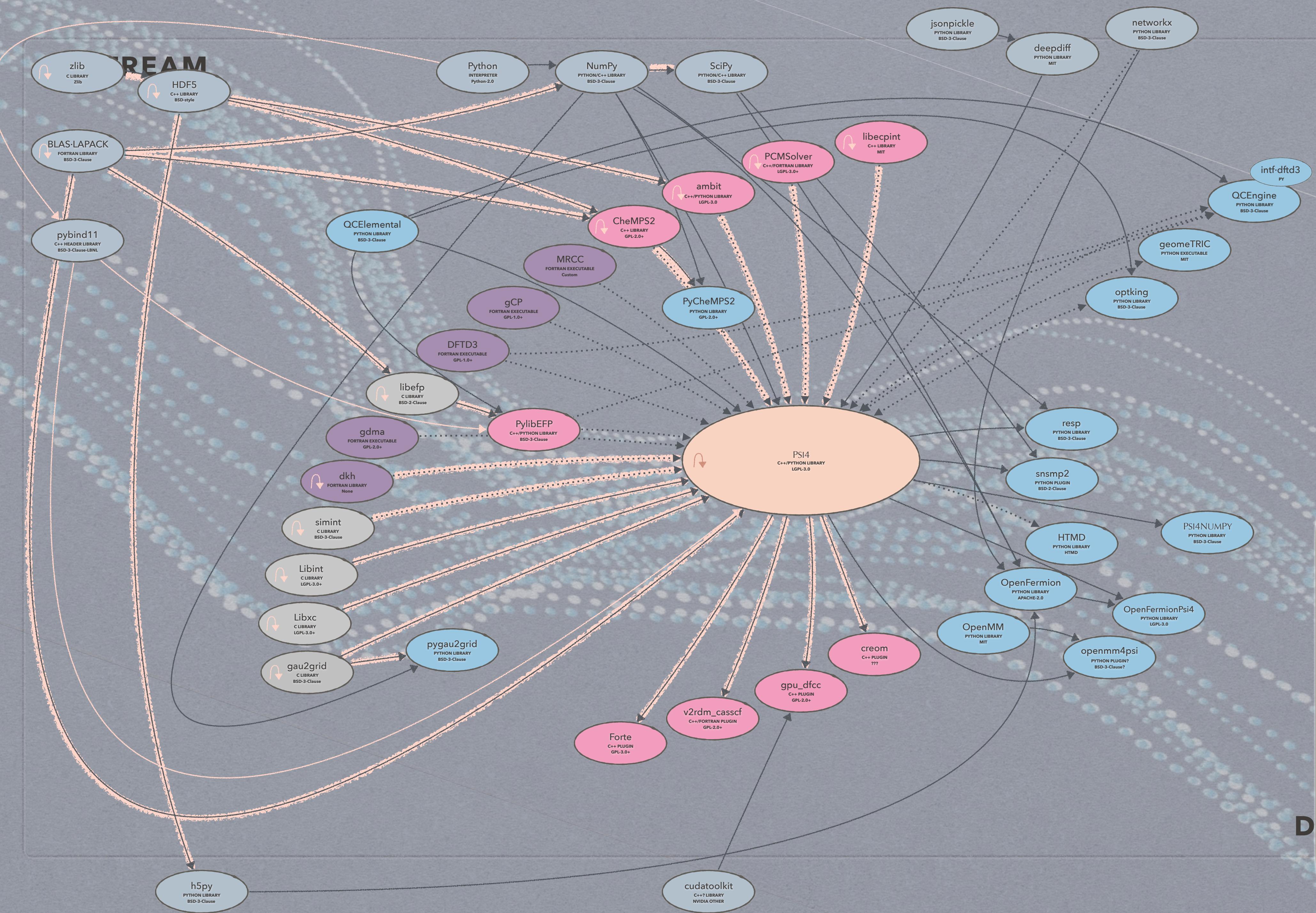
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Common Driv

- separate psi4.core from generic QC portions of driver

- former stays in psi4, latter becomes new frontend

- Psinthon won't change; PsiAPI aliases back to p4



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Themes

- de-monolithing our own code to be available to others from both upstream and downstream ends
- reshaping intf'es toward drop-in replacements
- moving light calc py-side

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