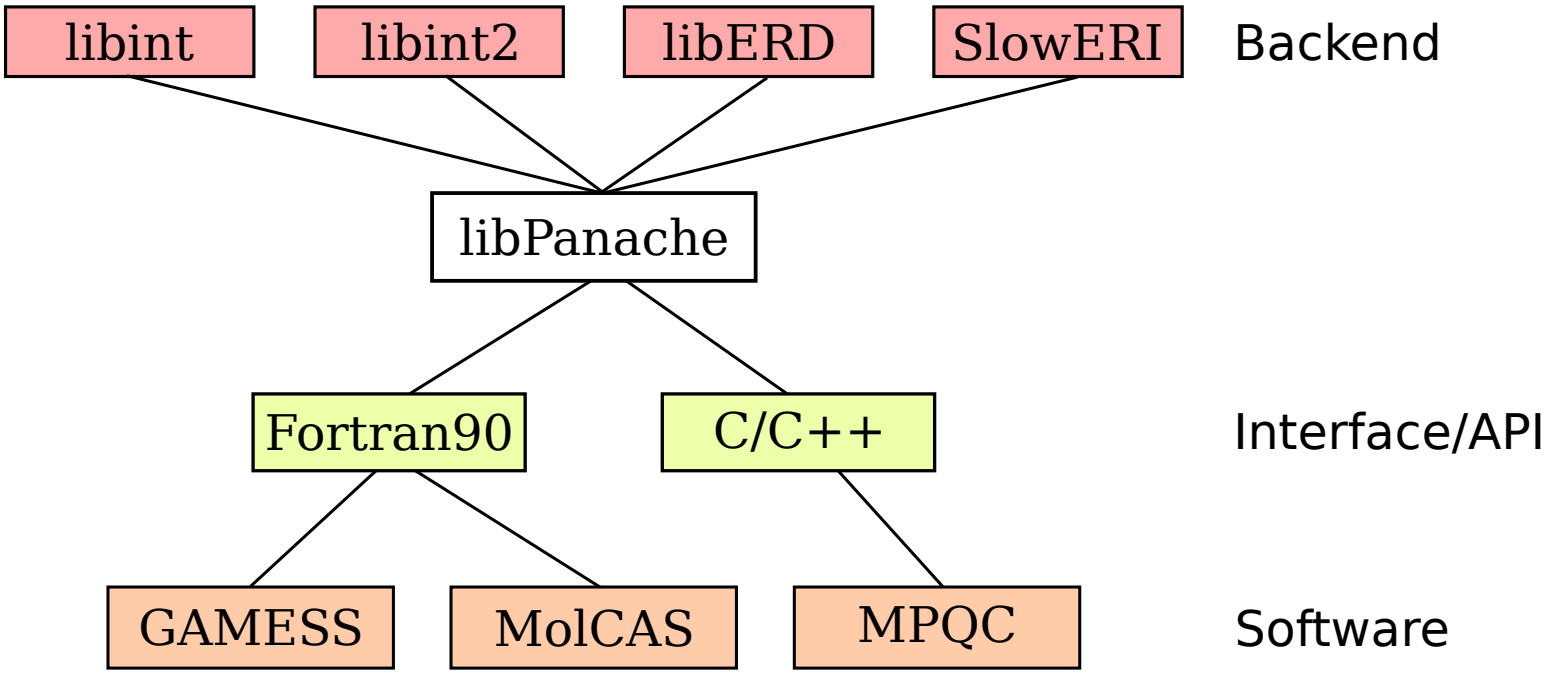
PANACHE

PArallel **N**umerical **A**pproximations in **Ch**emistry **E**ngine



Overview

- Library for 3-index approximations
  - Cholesky
  - Density Fitting
- C++ library
  - “Standard” C++
  - Minimal dependencies
  - C and Fortran interfaces

Current Features

- Calculation of Qso via density fitting or Cholesky decomposition
- C++/C/Fortran interface
- Transformations to Qmo, Qoo, etc.
- General interface for calculating & obtaining tensors
- Parallelized loops (OpenMP)
- Disk or memory based storage
- libint1, libint2, libERD backends
- Reordering & normalization
- Test implementation in GAMESS (MP2)

Current work: MPI/Cyclops

- Cyclops - distributed tensor library
- “Hard” part implemented - calculation of distributed Qso, and transformation to Qmo, etc.
- Harder part: Interface
  - Goal: Stop there, and hand back CTF Tensor objects to calling program
  - Problem: Cyclops does not have a C/Fortran interface

Solutions?

- C/Fortran tensor library?
  - Don't know of any
- Implement interface to CTF/TiledArray?
  - Beyond the scope of the project