TREX

NECI + TCHINT workflow

- TC-FCIQMC with NECI and TCHINT:

PYSCF

*.molden → CASINO

TCHINT ← parameters.casl

FCIDUMP (0,1,2-*e* ints)   TCDUMP (3-*e* ints)

NECI
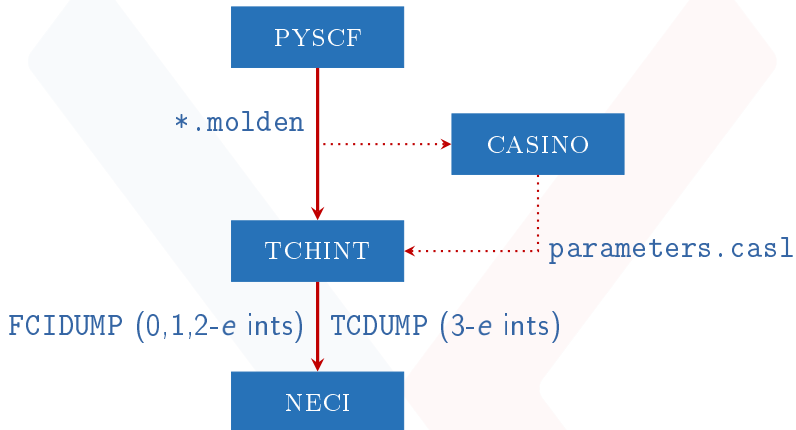
- TC method provides ~ 2 cardinal-number advantage: