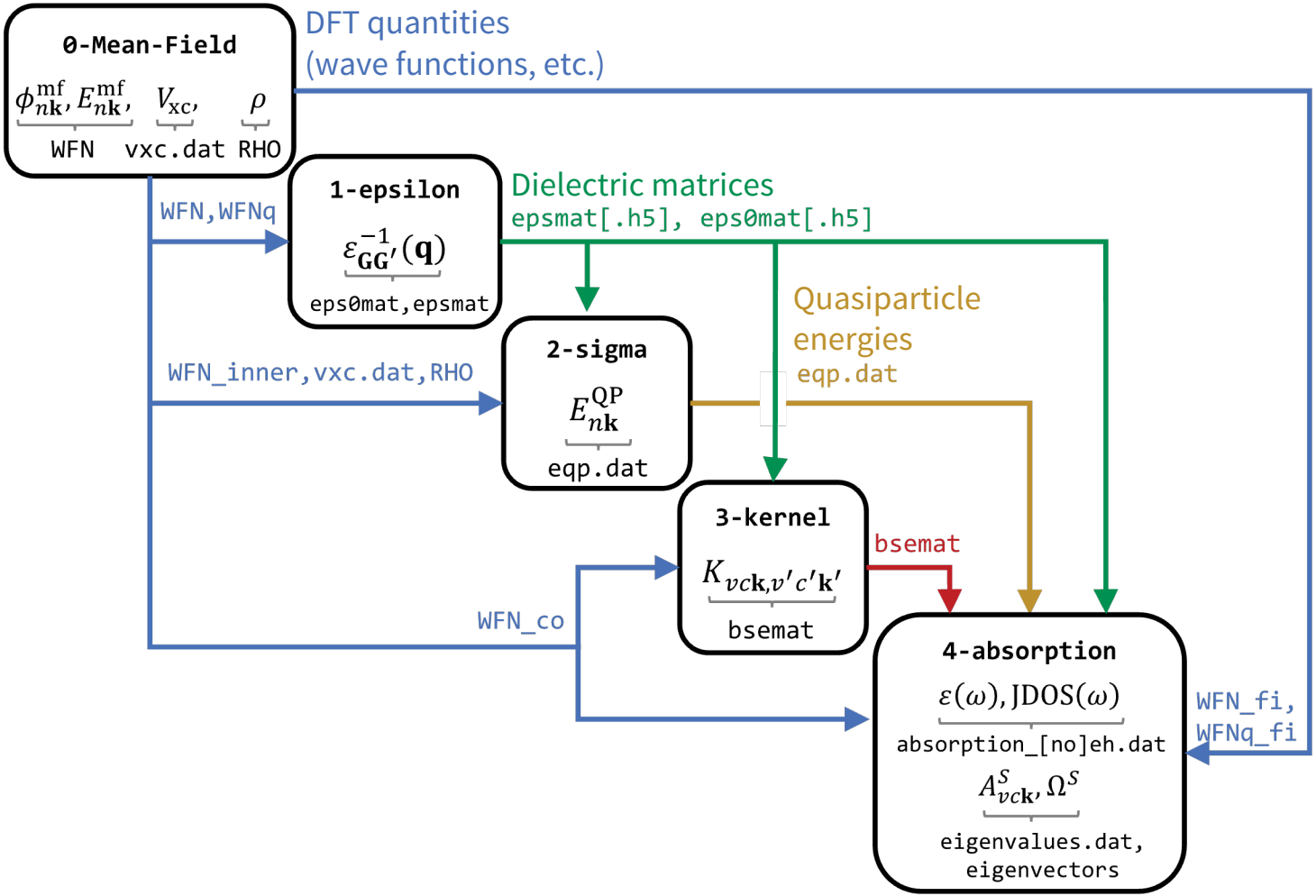
BerkeleyGW Hands-on Session: Computing the Optical Absorption Spectrum of Si

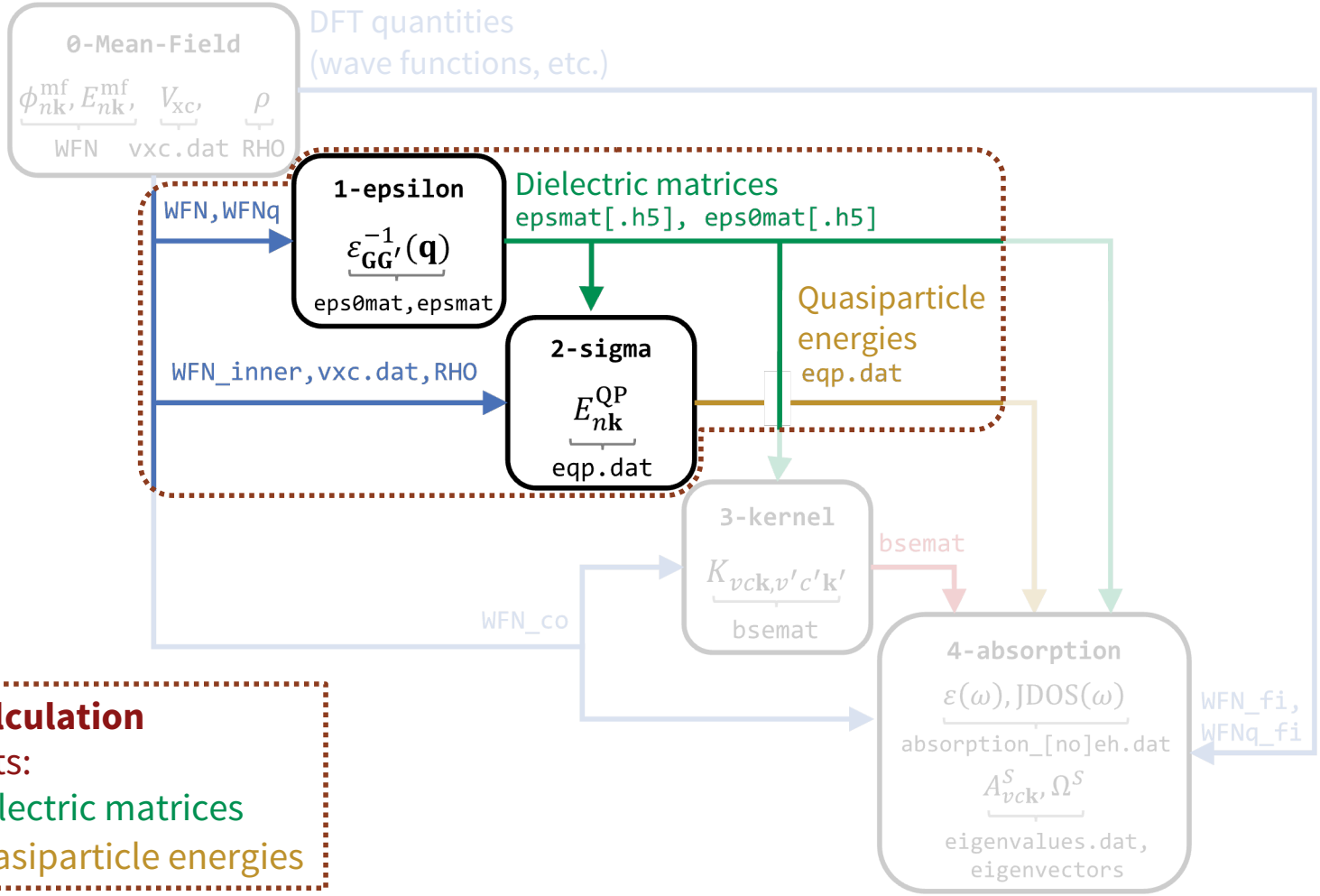
Felipe H. da Jornada
Department of Materials Science and Engineering, Stanford University
Stanford PULSE Institute, SLAC National Laboratory

Los Alamos Computational Condensed Matter Summer School 2025
June 20, 2025

Afternoon: hands-on session!

BerkeleyGW

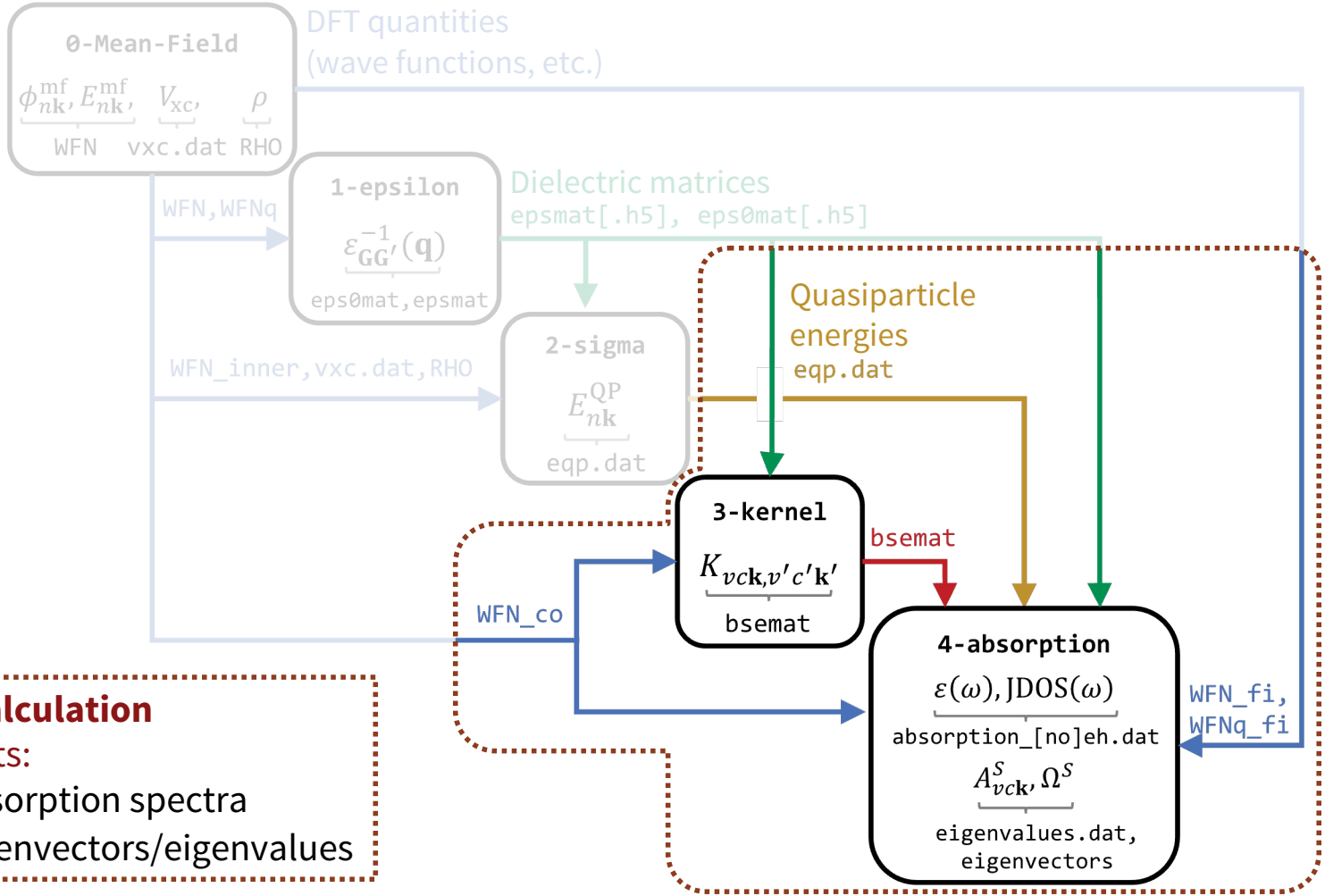

0-Mean-Field
$\phi^{mf}_{n\mathbf{k}}, E^{mf}_{n\mathbf{k}}$, V_{xc}, ρ
WFN vxc.dat RHO
DFT quantities
(wave functions, etc.)
WFN,WFNq
1-epsilon
$\varepsilon^{-1}_{\mathbf{GG}'}(\mathbf{q})$
eps0mat,epsmat
Dielectric matrices
epsmat[.h5], eps0mat[.h5]
WFN_inner,vxc.dat,RHO
2-sigma
$E^{QP}_{n\mathbf{k}}$
eqp.dat
Quasiparticle
energies
eqp.dat
3-kernel
$K_{vc\mathbf{k},v'c'\mathbf{k}'}$
bsemat
bsemat
WFN_co
4-absorption
$\varepsilon(\omega)$, JDOS(ω)
absorption_[no]eh.dat
$A^S_{vc\mathbf{k}}, \Omega^S$
eigenvalues.dat,
eigenvectors
WFN_fi,
WFNq_fi



GW calculation

Outputs:

- Dielectric matrices
- Quasiparticle energies

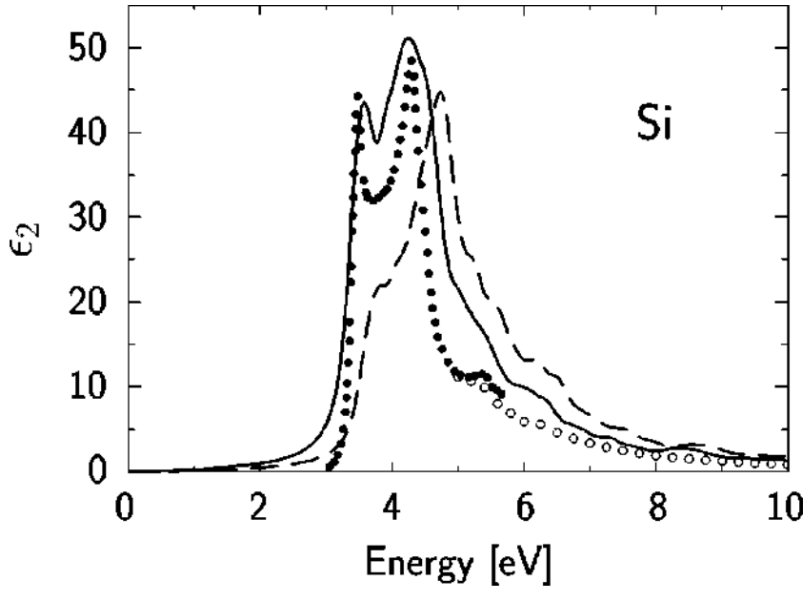


BSE calculation

Outputs:

- Absorption spectra
- Eigenvectors/eigenvalues

Hands-on Session – Absorption Spectrum of Silicon



M. Rohlfing, S. G. Louie, PRB **62**, 8 (2000).

- Goals:
  - Reproduce plots on the left
  - Partial convergence study wrt k-point sampling and number of bands
- Stretch goals:
  - Scissors operators
  - Local fields

Instructions:
https://berkeleygw.notion.site/