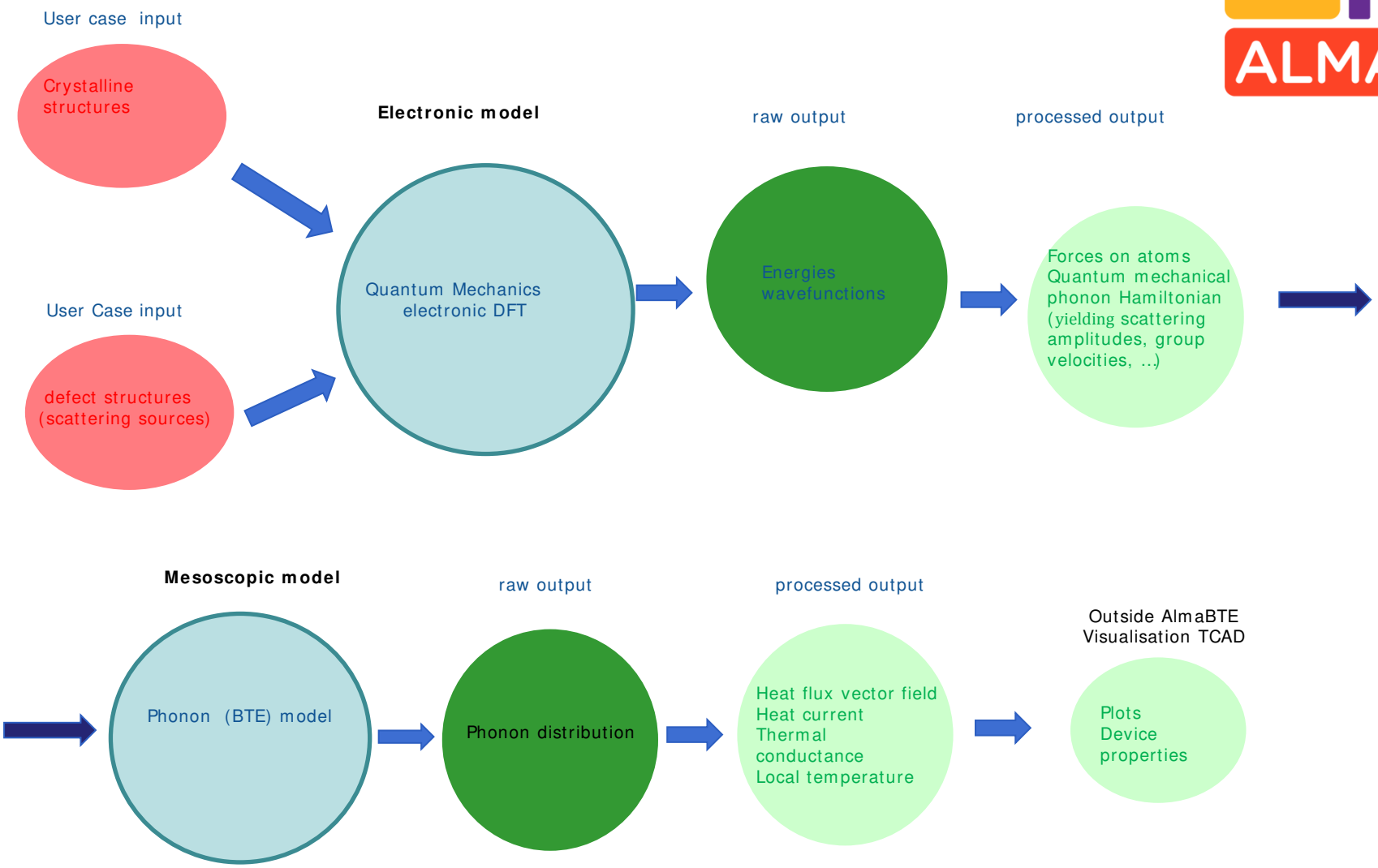
User case input
Crystalline structures
User Case input
defect structures (scattering sources)
Electronic model
Quantum Mechanics electronic DFT
raw output
Energies wavefunctions
processed output
Forces on atoms
Quantum mechanical phonon Hamiltonian (yielding scattering amplitudes, group velocities, ...)
Mesoscopic model
Phonon (BTE) model
raw output
Phonon distribution
processed output
Heat flux vector field
Heat current
Thermal conductance
Local temperature
Outside AlmaBTE
Visualisation TCAD
Plots
Device properties