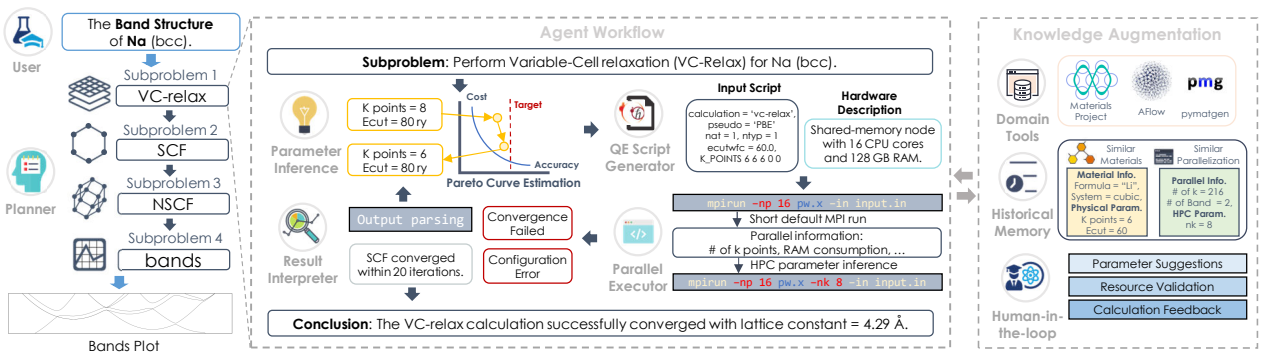
User
The Band Structure of Na (bcc).
Planner
Subproblem 1
VC-relax
Subproblem 2
SCF
Subproblem 3
NSCF
Subproblem 4
bands
Bands Plot
Agent Workflow
Subproblem: Perform Variable-Cell relaxation (VC-Relax) for Na (bcc).
Parameter Inference
K points = 8
Ecut = 80 ry
K points = 6
Ecut = 80 ry
Cost
Target
Accuracy
Pareto Curve Estimation
QE Script Generator
Input Script
calculation = 'vc-relax',
pseudo = 'PBE'
nat = 1, ntyp = 1
ecutwfc = 60.0,
K_POINTS 6 6 6 0 0 0
Hardware Description
Shared-memory node with 16 CPU cores and 128 GB RAM.
mpirun -np 16 pw.x -in input.in
Short default MPI run
Parallel information:
# of k points, RAM consumption, ...
HPC parameter inference
mpirun -np 16 pw.x -nk 8 -in input.in
Parallel Executor
Result Interpreter
Output parsing
Convergence Failed
SCF converged within 20 iterations.
Configuration Error
Conclusion: The VC-relax calculation successfully converged with lattice constant = 4.29 Å.
Knowledge Augmentation
Domain Tools
Materials Project
AFlow
pymatgen
Historical Memory
Similar Materials
Material Info.
Formula = "Li",
System = cubic,
Physical Param.
K points = 6
Ecut = 60
Similar Parallelization
Parallel Info.
# of k = 216
# of Band = 2,
HPC Param.
nk = 8
Human-in-the-loop
Parameter Suggestions
Resource Validation
Calculation Feedback