

Multi-step DFT Execution



Search Structural Information
(Web Search, Open Database)

Human

2 min~20 min

TritonDFT

5 s~1 min



Configure Physical Parameters
(Science Expertise)

Human

27 min~4 hour

TritonDFT

4 s~2 min



Write DFT Library Scripts
(Software Details)

Human

11 min~2 hour

TritonDFT

5 s~1 min



Job Submission & Parallelization
(HPC Expertise)

Human

5 min~10 min

TritonDFT

5 s~2 min



Log Parsing & Result Analysis
(Software + Science Expertise)

Human

15 min~3 hour

TritonDFT

4 s~5 min