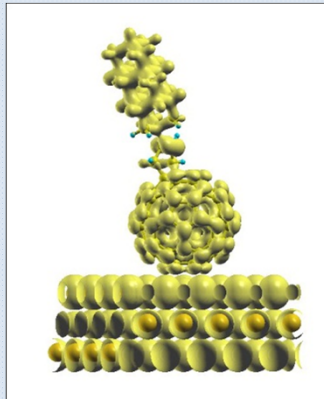# Computing capabilities and needs for simulations in photon science
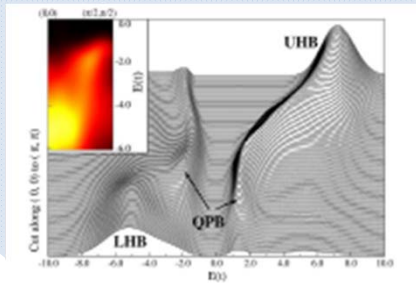
Lex Kemper

Computing needs by method:
"I need lots of…"
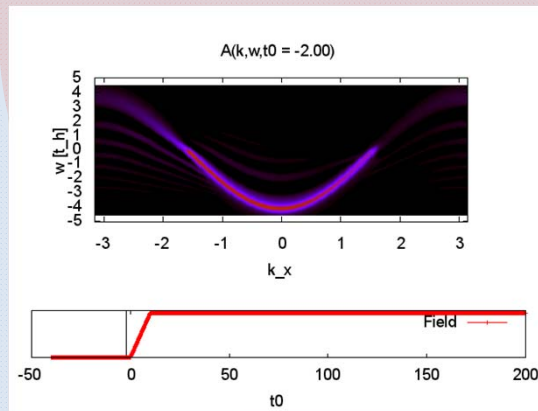

Density Functional Theory

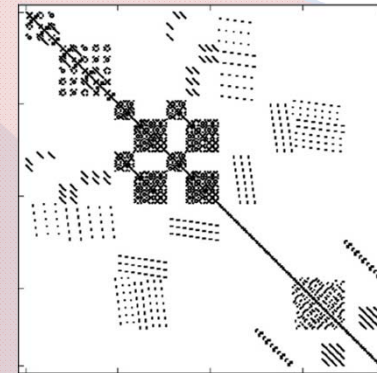Exact diagonalization

CPU TIME

MEMORY

Quantum Monte Carlo

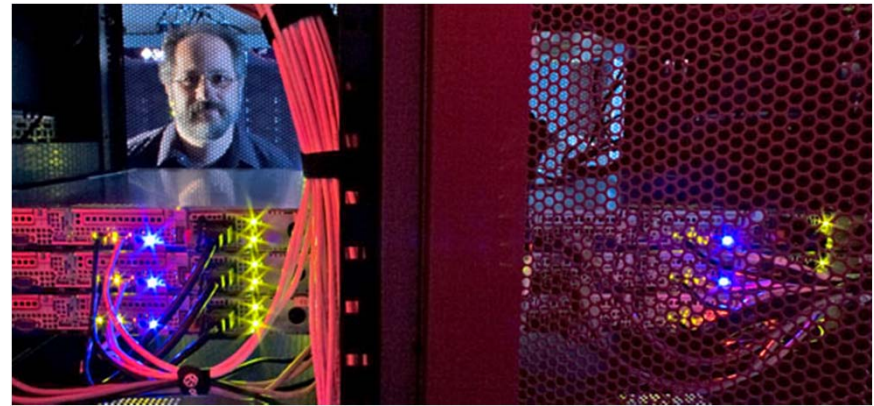Time domain spectroscopy

The needs are varied, so are the tools

- SIMES Cluster @ SLAC:
    - 64 nodes, 512 CPUs
    - 16G memory / node
    - Max performance ~ 5 Tflops
    - DDR Infiniband interconnect

- SIMES GPU Cluster @ SLAC
    - 5 nodes, 80 CPUs
    - NVidia GPU cards

- SIMES Cluster phase II @ SLAC:
    - 40 nodes, 240 CPUs
    - 48G memory / node
    - QDR Infiniband interconnect
    - Coming soon!

The needs are varied, so are the tools

SIMES CLUSTER @ SLAC

Jaguar (Cray XT5) @ Oak Ridge National Lab   #2

Hopper (Cray XE6) and Franklin (Cray XT4) @ NERSC

#5

Over 2 million hours!

#26

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