Space-Filling Curves for Real-Space Pseudopotential Density Functional Theory Calculations

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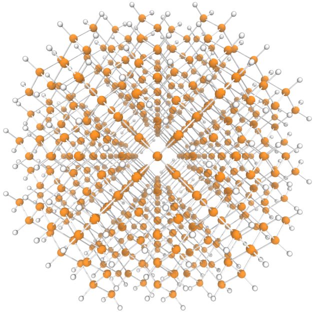
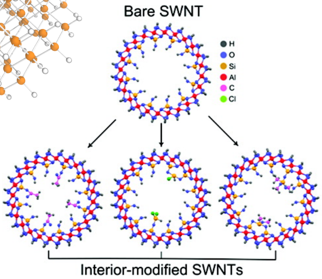
Motivation – electronic structure of large systems

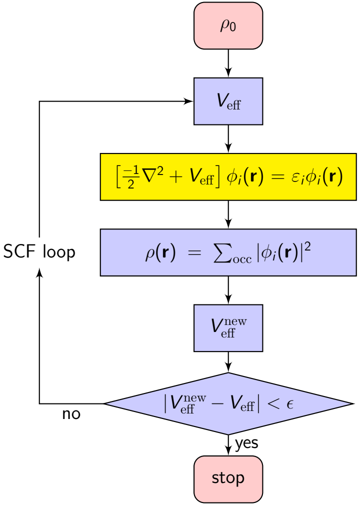
- Silicon nanocrystals
    - Optoelectronics
    - Quantum computers
    - 10 nm in diameter $\sim$ 20,000 atoms
- Nanotubes
    - Catalysis
    - Water desalination
    - 20 nm in length $\sim$ 5,000 atoms



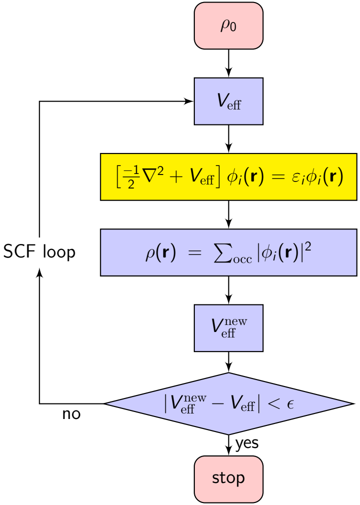


Kang, Zang, Jones, Nair, J Phys Chem C 115, 7676-7685 (2011)

Electronic structure from Kohn–Sham DFT

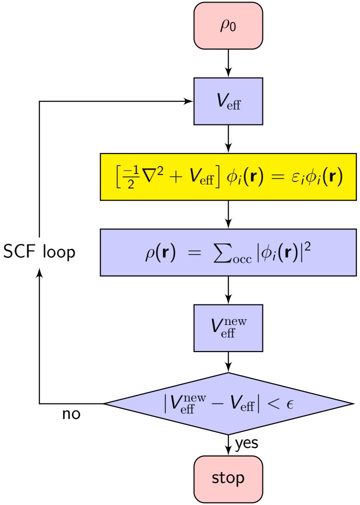


Electronic structure from Kohn–Sham DFT



Key to large systems:
An efficient eigensolver

Electronic structure from Kohn–Sham DFT

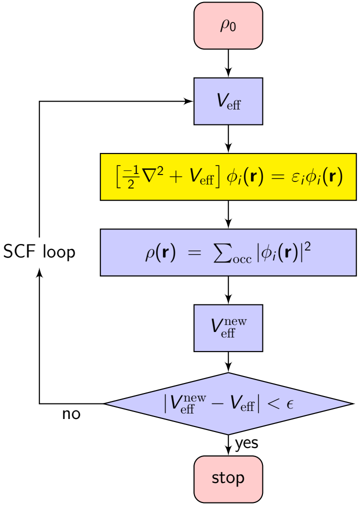


Key to large systems:
An efficient eigensolver

Observation

A converged charge density (rather than individual wfns) is enough to advance the SCF iteration

Electronic structure from Kohn–Sham DFT



Key to large systems:
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Chebyshev-filtered subspace iteration

1. Filtering
2. Orthonormalization
3. Rayleigh–Ritz refinement

Chebyshev filtering requires many MatVecs

- H is not stored, accessed via Hv

  H: Hamiltonian matrix

  v: wave functions

- Cost $\sim O(Nsm)$

  N: number of grid points

  s: number of states

  m: degree of the filter

- Faster $Hv \rightarrow$ more efficient eigensolver :)

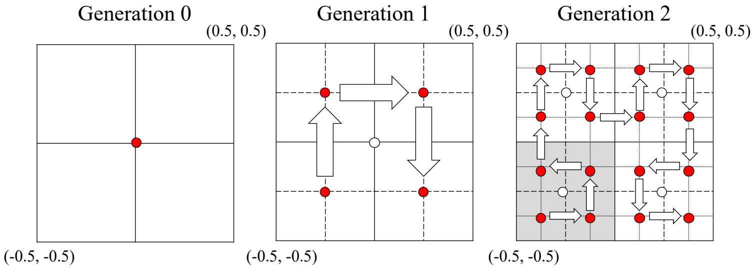
Algorithm 1 Chebyshev filtering

```
procedure W = CHEBYFILTER(H, V, m, ε_F, λ_ub, λ_lb)
    e = (λ_ub − ε_F)/2
    c = (λ_ub + ε_F)/2
    σ = e/(c − λ_lb)
    τ = 2/σ
    W = (HV − cV)(σ/e)
    for i = 2 → m do
        σ_new = 1/(τ − σ)
        W_t = (HV − cV)(2σ_new/e) − (σσ_new)V
        V = W
        W = W_t
        σ = σ_new
```

Liou, Yang, Chelikowsky, Comput Phys Commun 254, 107330 (2020)

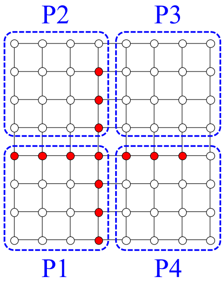
Space-filling curves for faster *Hv*

- One-dimensional representation of multi-dimensional space
- Self-similarity
- We use Hilbert space-filling curves

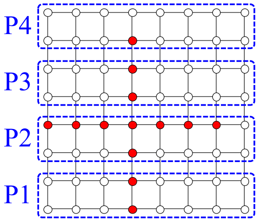


Space-filling curves for real-space grid partitioning

1. Good locality of grid points
   - Lower communication overhead
   - More load-balancing



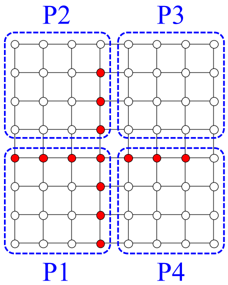
Partitioning using **Hilbert curves**



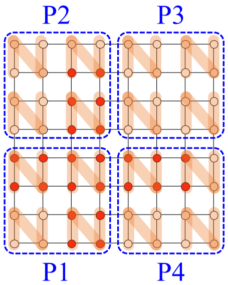
Partitioning using **simple Cartesian ordering (SCO)**

Space-filling curves for real-space grid partitioning

2. Use of grid blocks
   - Blockwise operations (vectorization)
   - More efficient indexing



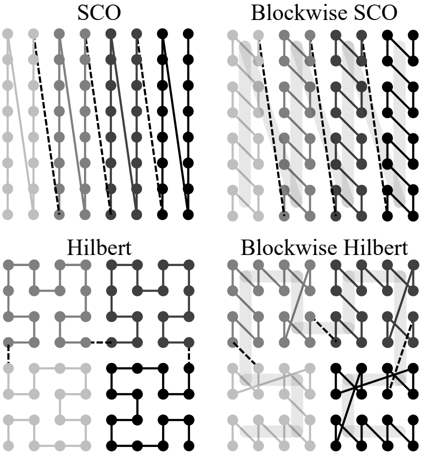
Without grid blocks



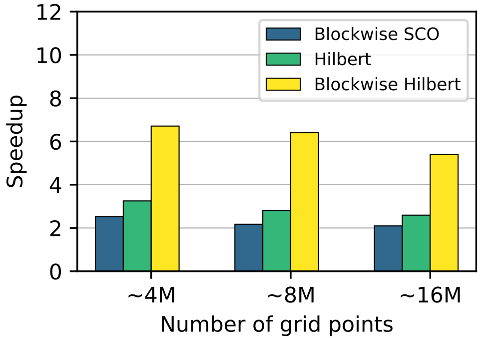
With grid blocks (blockwise)

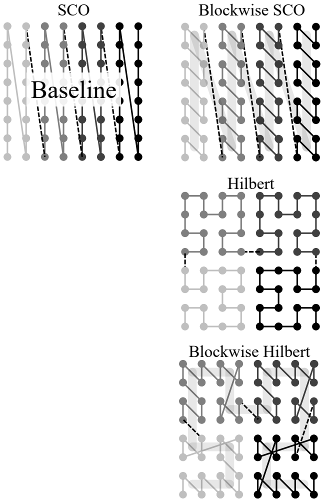
Four grid partitioning schemes

- Hilbert ordering or simple Cartesian ordering (SCO)
- non-blockwise or blockwise



Results – speedup

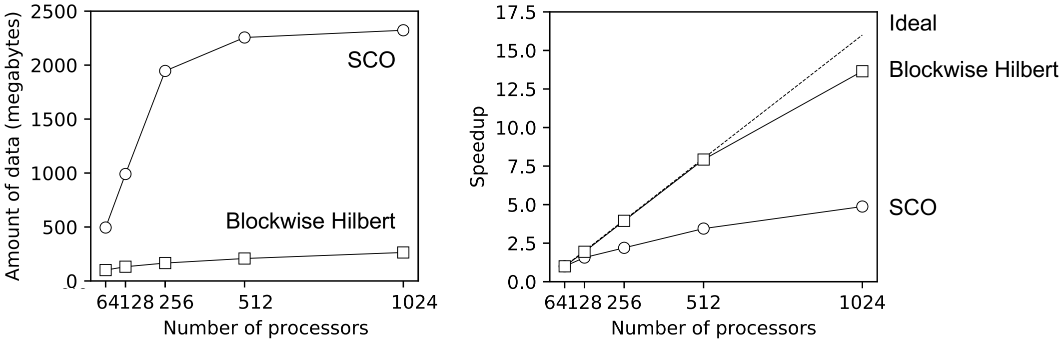




- Blockwise ops → improved vectorization
- Hilbert curves → improved communication

Liou, Biller, Kronik, Chelikowsky, submitted

Results – scalability

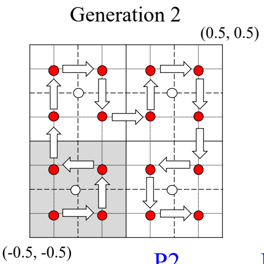


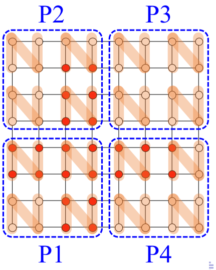
- Less data to transfer and more load-balancing
- Better scalability

Liou, Biller, Kronik, Chelikowsky, submitted

Summary

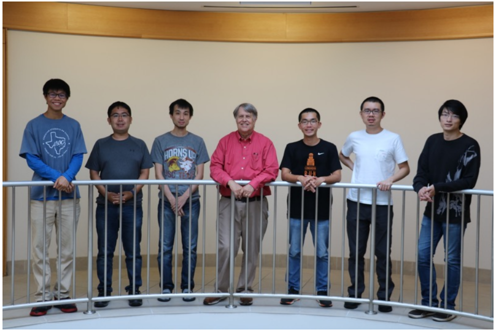
- Space-filling curves for real-space pseudopotential DFT calculations (e.g., PARSEC code)
  - **Hilbert curves**
  - **Blockwise opertions**
- **Reduced communication** between processors, increased opportunity for **vectorization**, and **improved scalability** of the filtering step





PARSEC (http://real-space.org/)

Acknowledgements



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