Solving the Schrödinger equation in parallel for large-scale systems

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Purpose & Problem

- Main purpose: Linear scaling methods for optical properties calculation
- Problem: Too many eigenstates

$$2 N_{unocc} + N_{occ}$$

- Folded Spectrum Method (FSM)

J. Chem. Phys. 100, 2394 (1994)

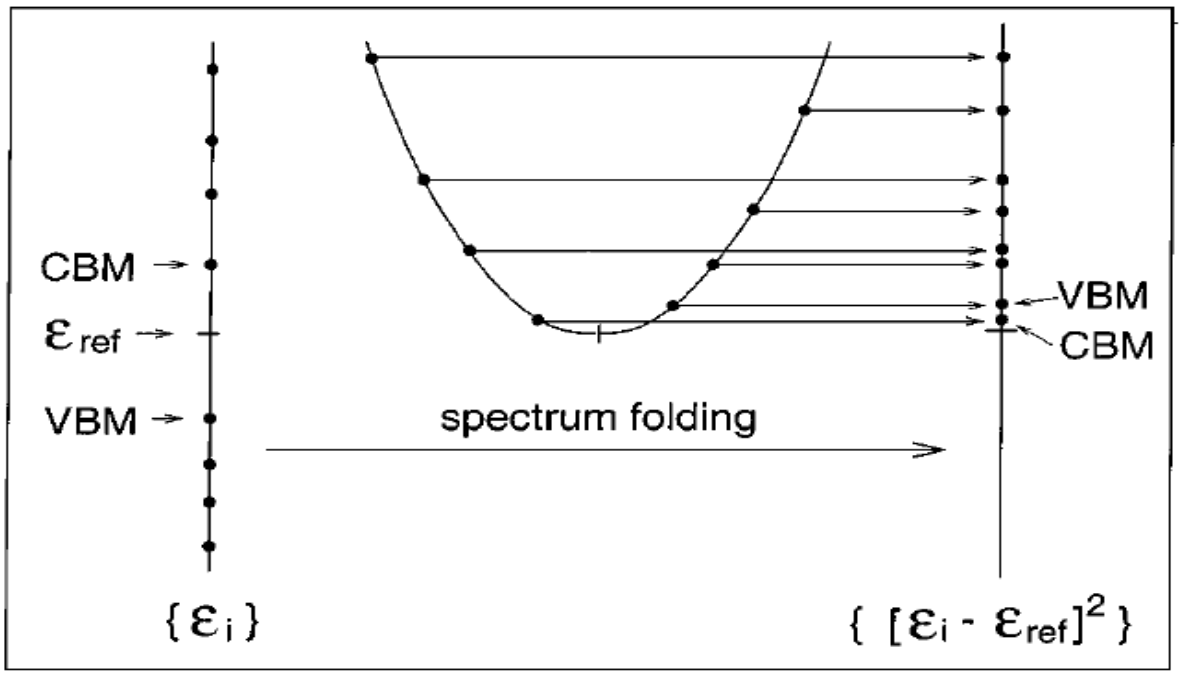
J. Comp. Phys. 160, 29 (2000)

FSM

$$\hat{H}\psi = \varepsilon\psi$$

$$\left(\hat{H} - \varepsilon_{ref}\right)^2 \psi = (\varepsilon - \varepsilon_{ref})^2 \psi$$

$$F = \left\langle \psi \left| (\hat{H} - \varepsilon_{ref})^2 \right| \psi \right\rangle$$



J. Comp. Phys. 160, 29 (2000)

Evaluation

- Successful in one dimensional DFT testing code

Eigenvalues solved by FSM in different energy windows

FSM	Exact
47.2701228576943	47.2701268780046
88.0007682096316	88.0007682096313
88.9937494024913	88.9937494024913
142.397939798585	142.397939798585
142.729909609642	142.729909060828

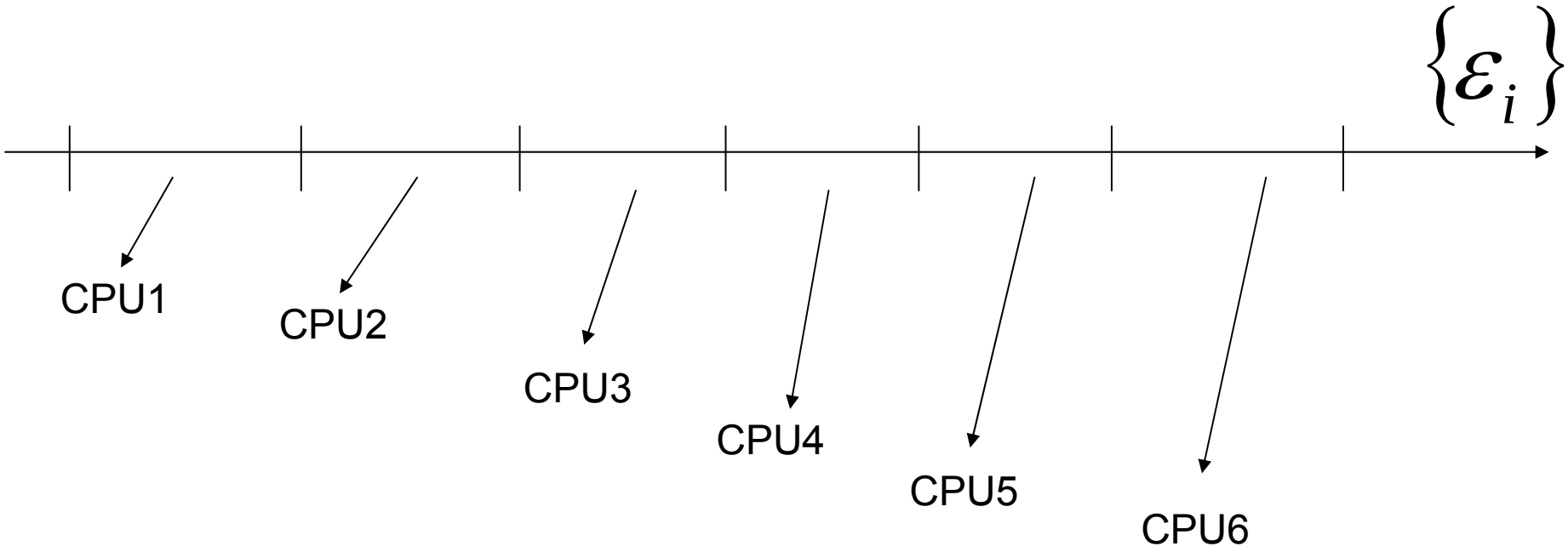
$\varepsilon_{ref} =$ 95 eV

FSM	Exact
2.41914682034080	2.41914682029973
16.9261093835735	16.9261093835728
17.0394992636753	17.0394992636757
45.8624070955793	45.8624070955796
47.2701268780026	47.2701268780046

$\varepsilon_{ref} =$ 15 eV

New Idea

- Divide and conquer solve the whole spectrum



Parallelization Tactics

- For few eigenstates: k-points or g-vectors distribution

  (save computational effort to do a lot of orthogonisation)

- For the whole spectrum: bands distribution

  (Each node only calculates its own energy window)

Conclusion

- A linear scaling method for optical properties calculation can be achieved by the two parallelization tactics either for the problem only concerns with the few states near band gap or for the problem needs to solve the whole spectrum.
- Successful in 1D case, still having some bugs in CASTEP code, implementing in ONETEP in the future