



Numerical methods for PDEs

How to approximate spatial derivatives?

Grid method

$$\frac{\partial f(x, t)}{\partial x} \Big|_{x=x_i} \approx \frac{f_{i+1}(t) - f_{i-1}(t)}{2\Delta x}$$

Spectral Method

$$f(x, t) = \sum_m^N f_m(t) \phi_m(x) \quad C^\infty \text{ Basis set}$$

CIP method
(Grid method)

Spatial derivatives are treated as independent variables

CIP-BS method
(Grid+Spectral method)

Basis Set

- C^K
- Local support
- Independent to problem

$$f(x, t) = \sum_{k=0}^K \sum_i^N f_i^k(t) \phi_{k,i}(x)$$

Basis set approach in the CIP method

Constraints

$$x_i : f_i, f'_i, \dots, f_i^{(K)}$$

$$x_{i+1} : f_{i+1}, f'_{i+1}, \dots, f_{i+1}^{(K)}$$

Approximation

$$f(x) = \sum_{k=0}^K \sum_i^N f_i^{(k)} \phi_{k,i}(x)$$

Basis set

$$\phi_{k,i}(x) = (\theta(x - x_{i-1}) - \theta(x - x_i)) \phi_{k,i-}(x) + (\theta(x - x_i) - \theta(x - x_{i+1})) \phi_{k,i+}(x)$$

$\phi_{k,i-}(x), \phi_{k,i+}(x)$: Polynomial of degree $(2K+1)$

$$D_x^l \phi_{k,i-}(x_i) = \begin{cases} 1 & k=l \\ 0 & \text{otherwise} \end{cases}$$

$$D_x^l \phi_{k,i-}(x_{i-1}) = 0$$

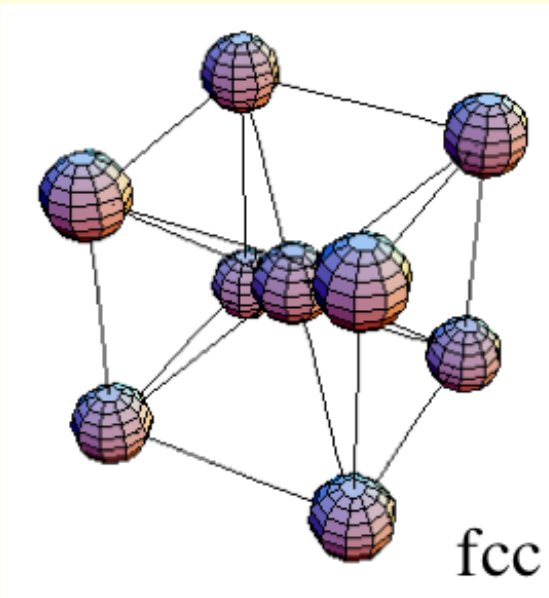
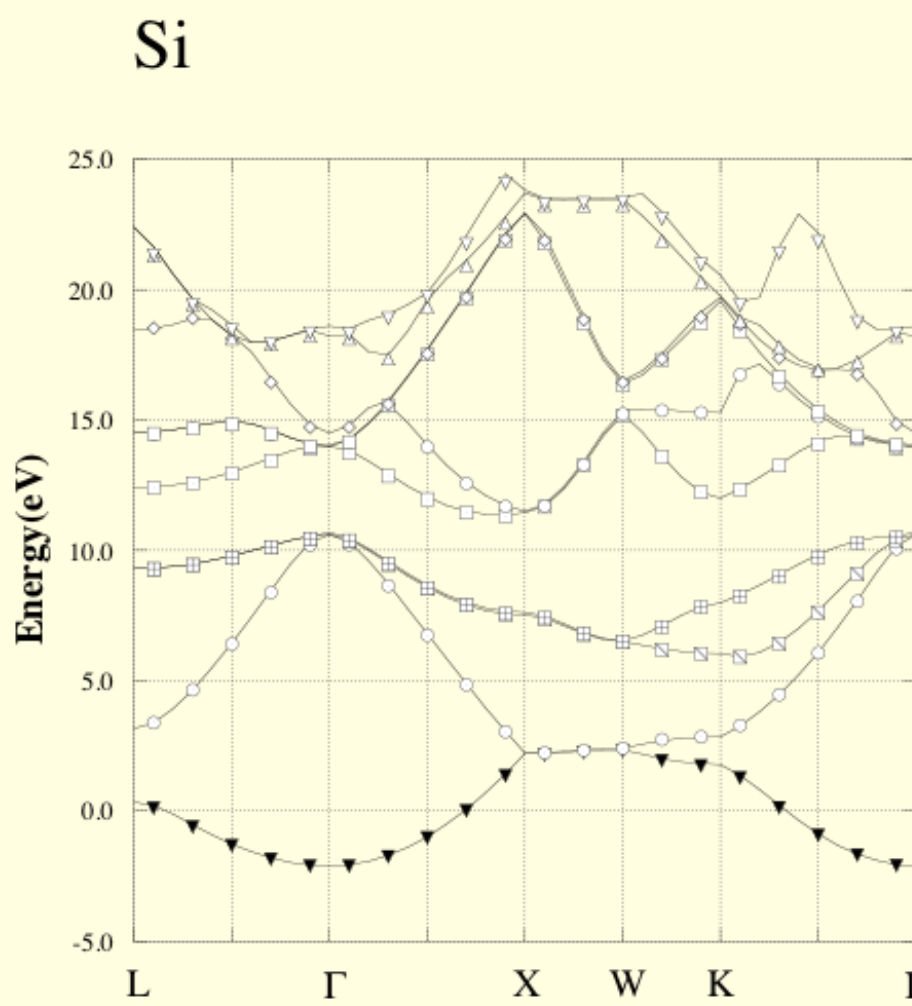
$$D_x^l \phi_{k,i+}(x_i) = \begin{cases} 1 & k=l \\ 0 & \text{otherwise} \end{cases}$$

$$D_x^l \phi_{k,i+}(x_{i+1}) = 0$$

$$l \leq K \quad D_x^l = \frac{\partial^l}{\partial x^l}$$

CIP-BS^K method

Electronic Band Structure



$$a = 10.261$$

$$\begin{matrix} V_3^S = -0.21 & V_3^A = 0 \\ V_8^S = +0.04 & V_4^A = 0 \\ V_{11}^S = +0.08 & V_{11}^A = 0 \end{matrix}$$

No. of Elements = 3X3X3

symbols: PW method

Discretization of PDEs

Time-dependent PDE

$$\frac{\partial}{\partial t} f(x, t) = L[f(x, t)]$$

Solution

$$f(x, t) = \sum_{k=0}^K \sum_i^N f_i^{(k)}(t) \phi_{k,i}(x)$$

Requirement: Residue must be orthogonal to each basis

$$\langle \phi_n | \frac{\partial}{\partial t} f(x, t) - L[f(x, t)] \rangle = 0$$

$$S \frac{d}{dt} f(t) = L[f(t)]$$

ODE

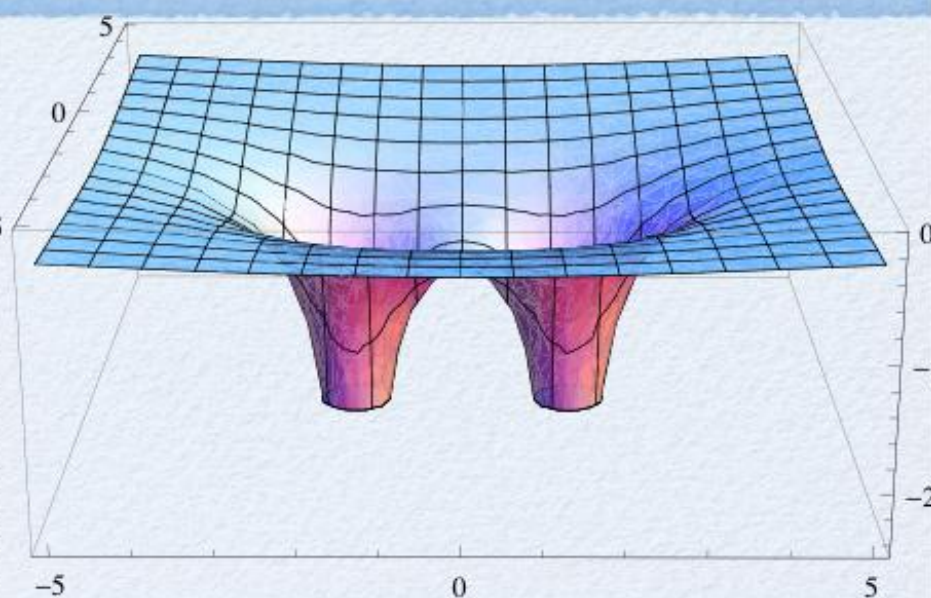
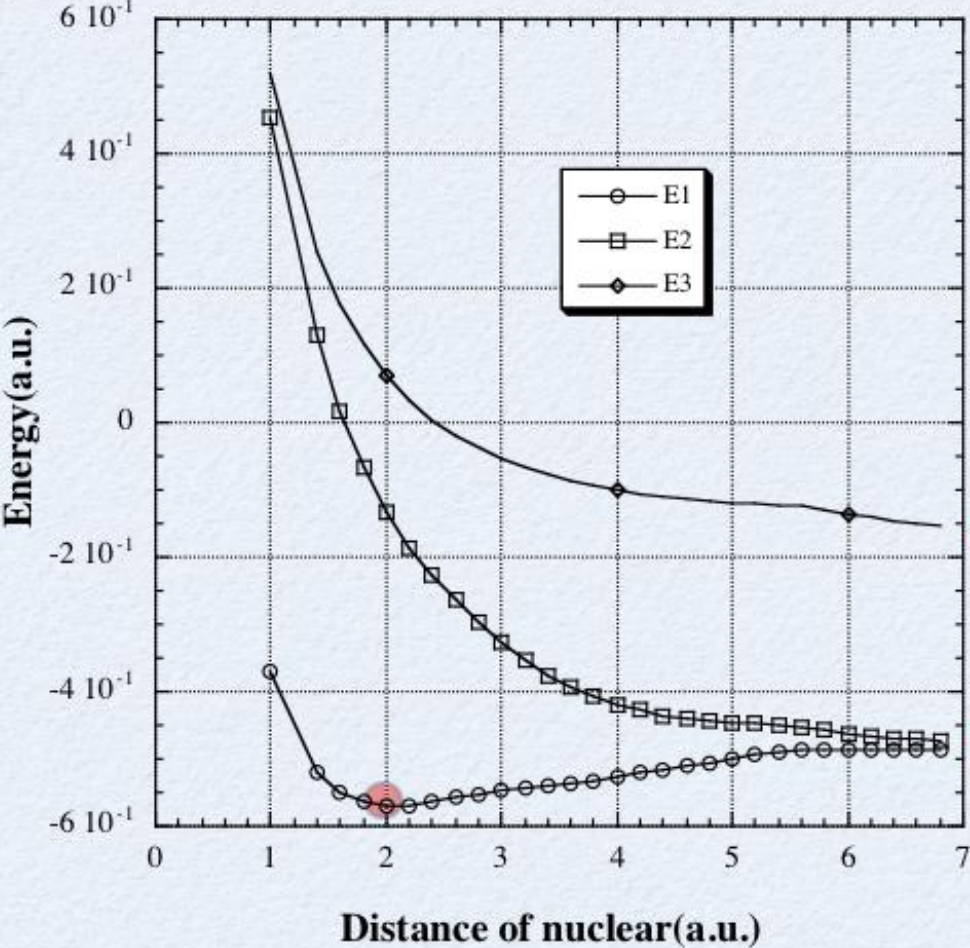
L : operator

S : Sparse, Symmetric, Non-singular, Banded Matrix

Molecular Electronic Structure

$$\Delta V(\mathbf{r}) = \delta(\mathbf{r} - \mathbf{a}) + \delta(\mathbf{r} + \mathbf{a})$$

$$\left(-\frac{1}{2}\nabla^2 + V(\mathbf{r})\right)\varphi(\mathbf{r}) = E\varphi(\mathbf{r})$$



calculated measured

distance of nuclear 0.106nm
2.00a. u. = 2.00a. u.

energy of ground state -16.38eV
0.570a. u. = 0.602a. u.