

From wavelet theory to the BigDFT code

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History

- I. Daubechies, Orthonormal bases of compactly supported wavelets, *Comm. Pure and Appl. Math.*, 41 (7), pp. 909-996, 1988 (over 6000 citations)
- Orthonormal Wavelet Bases for Quantum Molecular Dynamics, C. J. Tymczak and Xiao-Qian Wang, *Phys. Rev. Lett.* 78, 3654 (1997)
- A. I. Neelov and S. Goedecker, *J. of. Comp. Phys.* **217**, 312-339 (2006)
- Daubechies wavelets as a basis set for density functional pseudopotential calculations, Luigi Genovese, Alexey Neelov, Stefan Goedecker, Thierry Deutsch, Alireza Ghasemi, Oded Zilberberg, Anders Bergman, Mark Rayson and Reinhold Schneider, *J. Chem. Phys.* 129, 014109 (2008)

Basis sets for electronic structure?

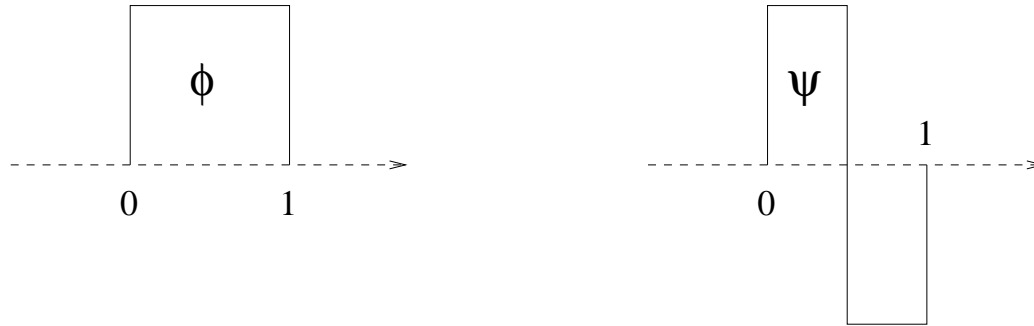
Plane waves:

- Operator approach: no need to set up Hamiltonian matrix
- FFT allows for quasi linear $M \log(M)$ scaling where M is number of plane waves
- Localization in Fourier space allows for efficient preconditioning techniques. Hence number of iterations independent of M
- Systematic convergence properties
- No localization in real space. Empty regions have to be filled with plane waves
- $O(N)$ scaling hard to achieve
- Resolution cannot adaptively be refined around the nucleus. All electron calculations impossible, hard pseudopotentials difficult.

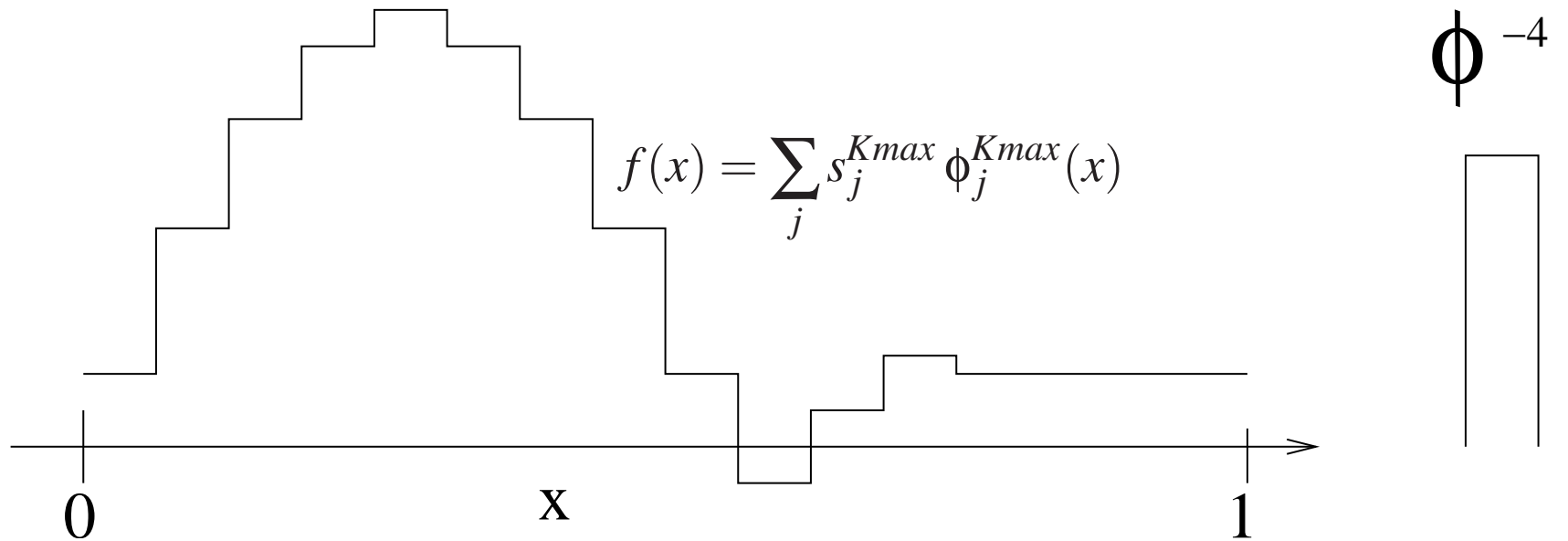
Gaussians:

- Small number of basis functions necessary for moderate accuracy (but much larger number of grid points)
- Real space localization makes them well suited for molecules and other open structures.
- Kinetic and overlap matrix elements can be calculated analytically.
- Good description of core electrons.
- No systematic convergence. Over-completeness before convergence. This leads also to problems with $O(N)$.
- Many different recipes for generating basis sets.
- Problematic for nanostructure.

Haar wavelet ψ and scaling function ϕ



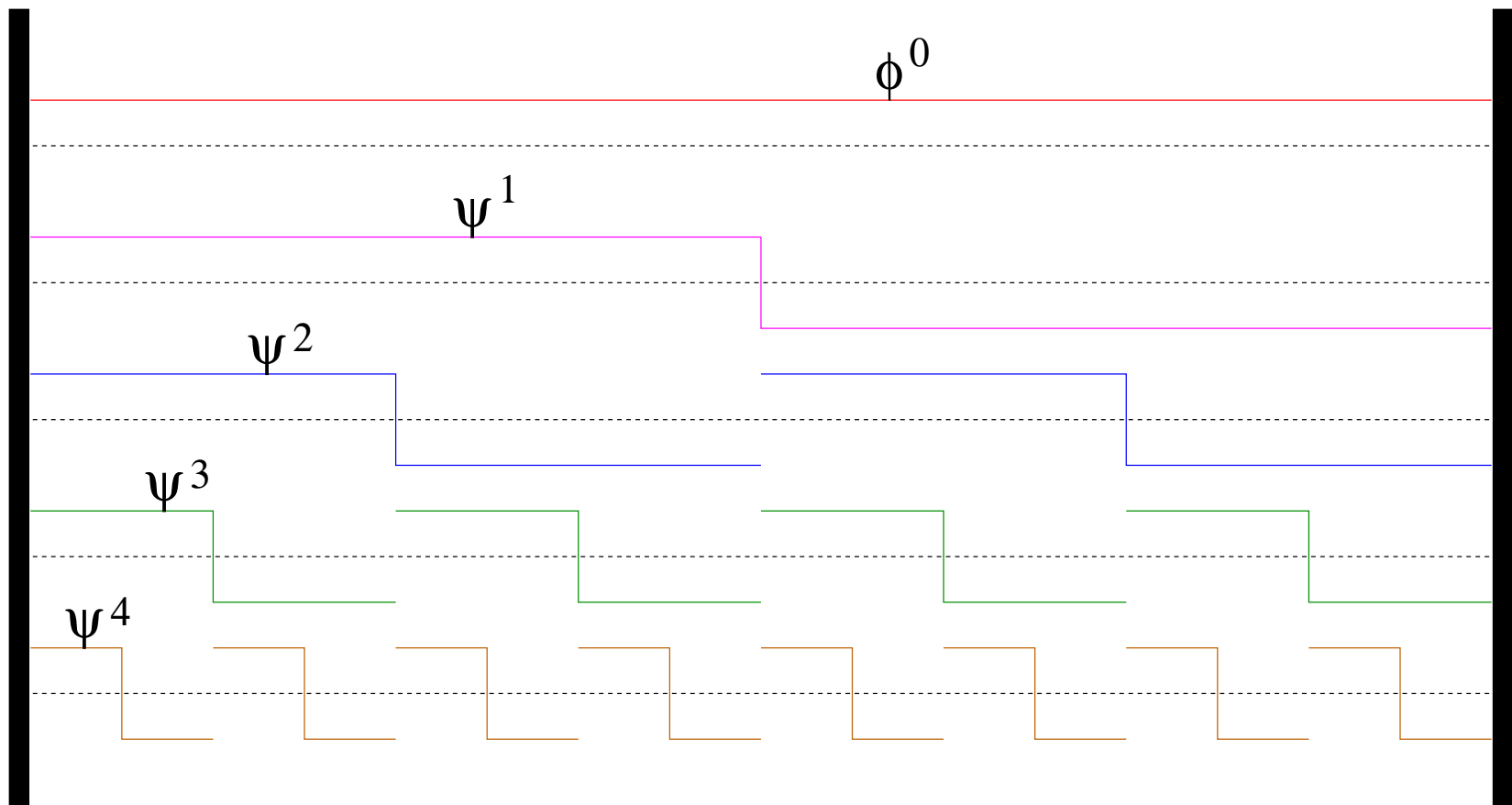
Scaling function representation



Refinement relations:

$$\phi(x) = \sum_{j=-m}^m h_j \phi(2x - j)$$

Haar wavelet basis set



Wavelet representation in general

$$f(x) = \sum_j s_j^{Kmin} \phi_j^{Kmin}(x) + \sum_{k=Kmin}^{Kmax} \sum_j d_j^k \psi_j^k(x)$$

Wavelet basis sets in three dimensions

1 scaling function

7 wavelets

all are products of 1-dim scaling functions and wavelets

$$\phi_{i,j,k}(x,y,z) = \phi(x-i)\phi(y-j)\phi(z-k)$$

$$\psi_{i,j,k}^1(x,y,z) = \phi(x-i)\phi(y-j)\psi(z-k)$$

$$\psi_{i,j,k}^2(x,y,z) = \phi(x-i)\psi(y-j)\phi(z-k)$$

$$\psi_{i,j,k}^3(x,y,z) = \phi(x-i)\psi(y-j)\psi(z-k)$$

$$\psi_{i,j,k}^4(x,y,z) = \psi(x-i)\phi(y-j)\phi(z-k)$$

$$\psi_{i,j,k}^5(x,y,z) = \psi(x-i)\phi(y-j)\psi(z-k)$$

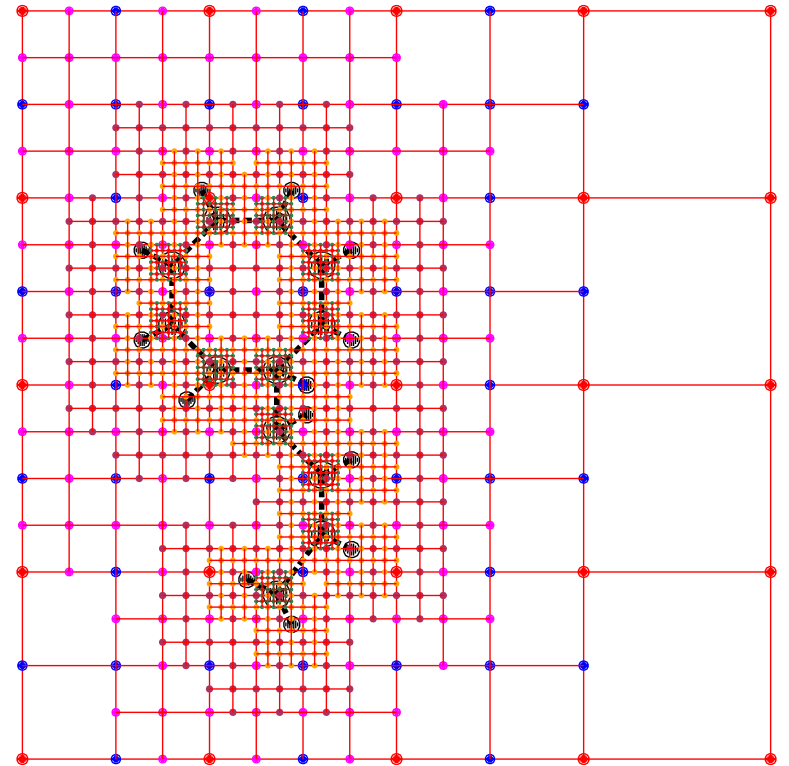
$$\psi_{i,j,k}^6(x,y,z) = \psi(x-i)\psi(y-j)\phi(z-k)$$

$$\psi_{i,j,k}^7(x,y,z) = \psi(x-i)\psi(y-j)\psi(z-k)$$

Wavelet basis sets

Properties of wavelet basis sets:

- localized both in real and in Fourier space
- allow for adaptivity

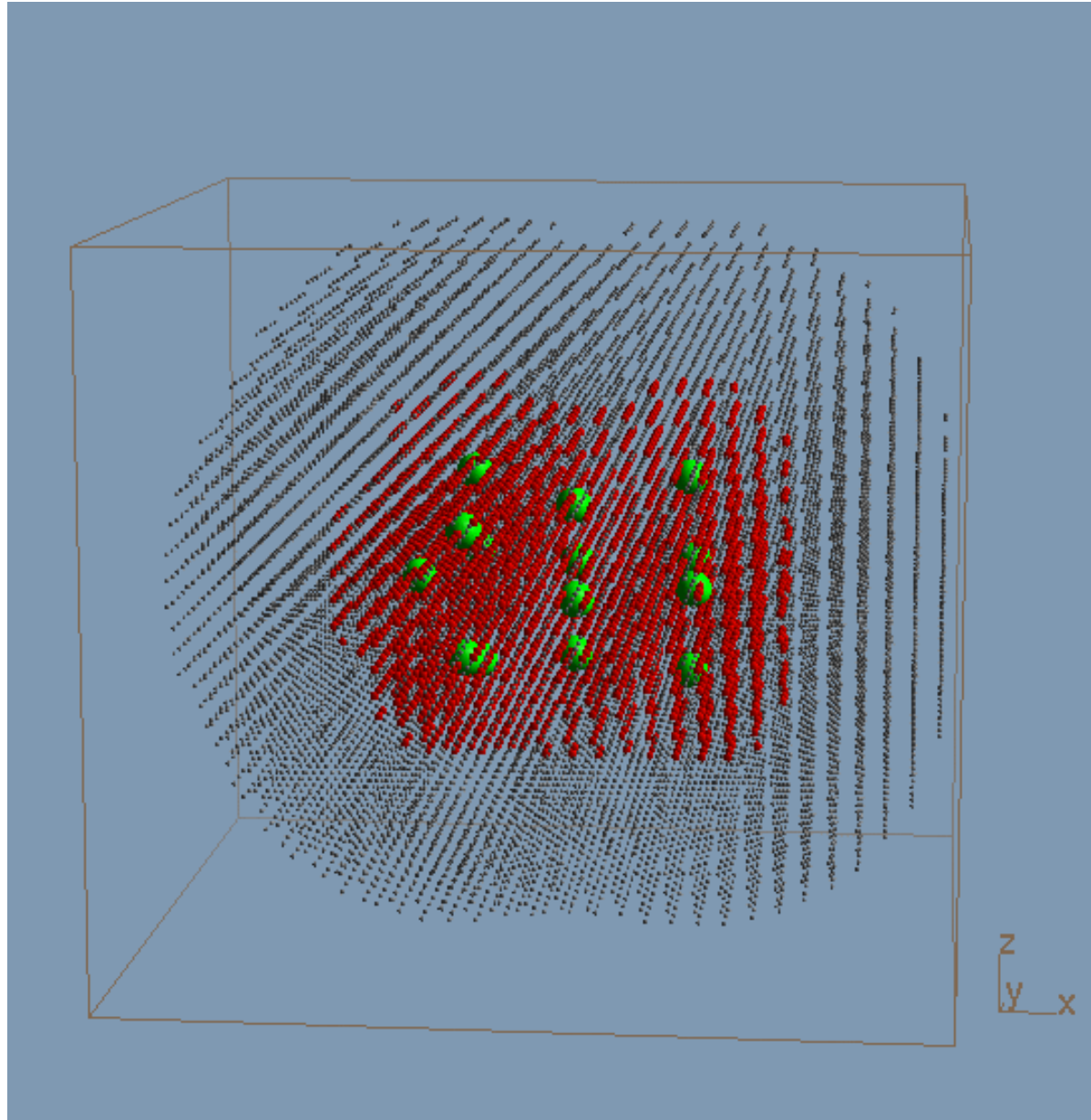


- are a systematic basis set

Basic choices in the BIGDFT code

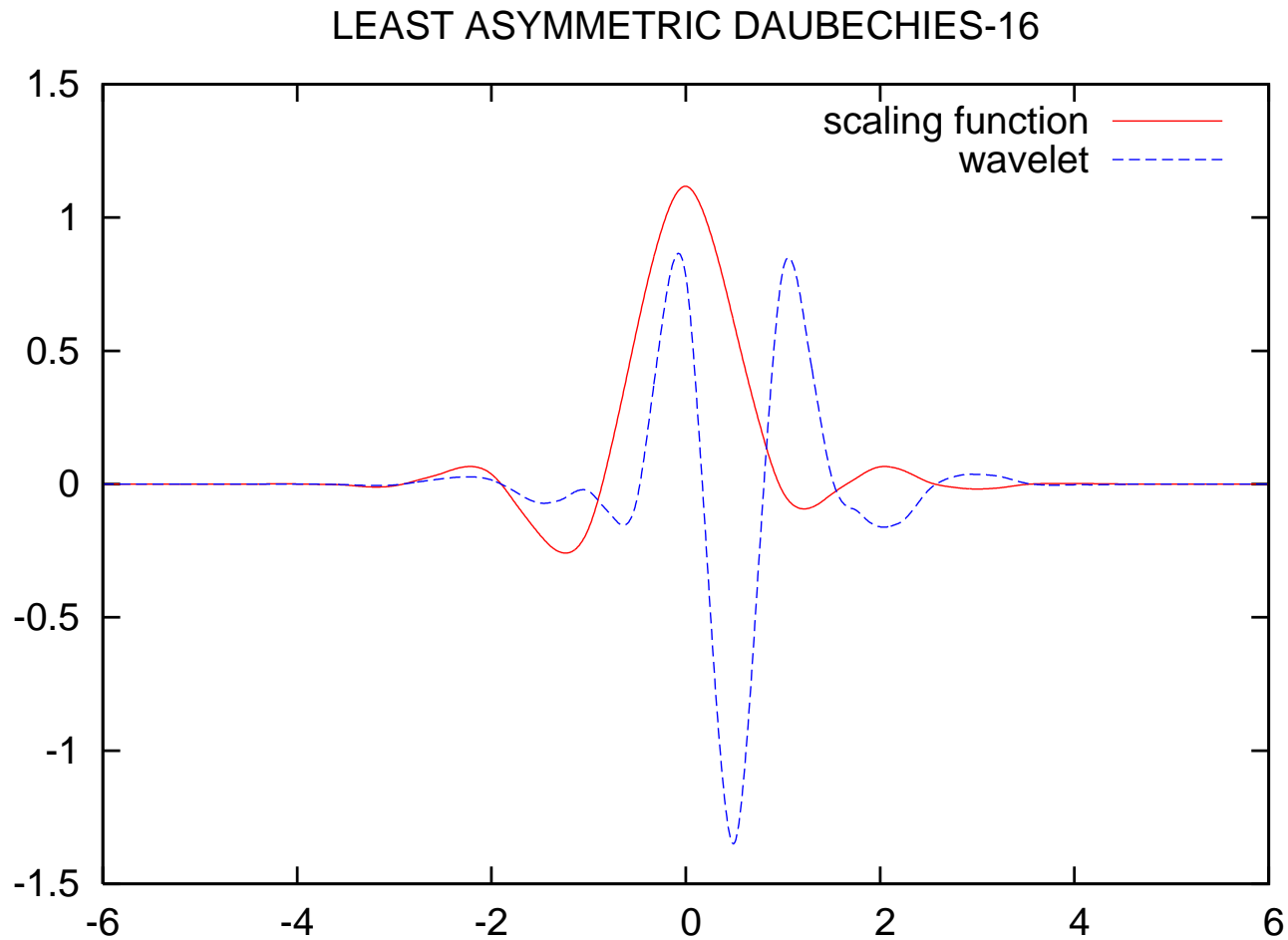
- Pseudopotentials are used
 - Pseudopotentials eliminate the chemically inactive core electrons and reduce thus the number of electron orbitals
 - Pseudopotentials are the simplest way to introduce relativistic effects into a non-relativistic calculation
 - The pseudopotential approximation is less severe than the approximate nature of the exchange correlation functional

- Only 2 resolution levels are used: simple adaptivity



High order Daubechies wavelets are used to represent wavefunctions

- orthogonality is very helpful (orthogonalization, nonlocal pseudopotential)
- Can represent exactly high degree polynomials (8-th order)



Basic relations for orthogonal wavelets

- An orthogonal wavelet family of degree m is characterized by 2 finite filters denoted by h_j, g_j , satisfying the orthogonality relations

$$\sum_l h_{l-2i} h_{l-2j} = \delta_{i,j},$$

$$\sum_l g_{l-2i} g_{l-2j} = \delta_{i,j},$$

$$\sum_l h_{l-2i} g_{l-2j} = 0$$

and the symmetry relation

$$g_{i+1} = (-1)^{i+1} h_{-i}.$$

- The refinement relations are

$$\phi(x) = \sqrt{2} \sum_{j=-m}^m h_j \phi(2x - j),$$

$$\psi(x) = \sqrt{2} \sum_{j=-m}^m g_j \phi(2x - j).$$

Orthogonality relations for a orthogonal wavelet basis

$$\begin{aligned}\int \phi(2^k x - i)\phi(2^k x - j)dx &= \delta_{i,j}, \\ \int \psi(2^k x - i)\phi(2^q x - j)dx &= 0, k \geq q, \\ \int \psi(2^k x - i)\psi(2^q x - j)dx &= \delta_{k,q}\delta_{i,j}.\end{aligned}$$

Expanding a function in an orthogonal wavelet basis

$$f(x) = \sum_i c_i \phi(x - i)$$

From orthogonality relation it follows

$$c_j = \int f(x)\phi(x - j)dx$$

Basic types of operations

- Application of the Kohn-Sham Hamiltonian on the wavefunctions (expressed in Daubechies)
 - Kinetic energy
 - Separable pseudopotential energy
 - Potential energy
- Orthogonalization and orthogonality constraints

$$\begin{aligned}\langle \Psi_i | \Psi_j \rangle &= \int \left(\sum_k C_k^i \phi(\mathbf{x} - k) \right) \left(\sum_l C_l^j \phi(\mathbf{x} - l) \right) d\mathbf{x} \\ &= \sum_k C_k^i C_k^j\end{aligned}$$

- Calculation of Hartree potential using interpolating scaling functions

Kinetic energy matrix elements between scaling functions

$$a_i = \int \phi(x) \frac{\partial^2}{\partial x^2} \phi(x-i) dx$$

Can be calculated exactly (Beylkin):

$$\begin{aligned} a_i &= \int \phi(x) \frac{\partial^2}{\partial x^2} \phi(x-i) dx \\ &= \sum_{\nu, \mu} 2h_\nu h_\mu \int \phi(2x - \nu) \frac{\partial^2}{\partial x^2} \phi(2x - 2i - \mu) dx \\ &= \sum_{\nu, \mu} 2h_\nu h_\mu 2^{2-1} \int \phi(y - \nu) \frac{\partial^2}{\partial y^2} \phi(y - 2i - \mu) dy \\ &= \sum_{\nu, \mu} h_\nu h_\mu 2^2 \int \phi(y) \frac{\partial^2}{\partial y^2} \phi(y - 2i - \mu + \nu) dy \\ &= \sum_{\nu, \mu} h_\nu h_\mu 2^2 a_{2i - \nu + \mu} \end{aligned}$$

We thus have to find the eigenvector \mathbf{a} associated with the eigenvalue of 2^{-2} ,

$$\sum_j A_{i,j} a_j = \left(\frac{1}{2}\right)^2 a_i$$

where the matrix $A_{i,j}$ is given by

$$A_{i,j} = \sum_{\nu,\mu} h_\nu h_\mu \delta_{j,2i-\nu+\mu}$$

Operator approach: Applying the kinetic energy operator results in a convolution with the filter a

$$(K\Psi)_i = \sum_j \Psi_j a_{i-j}$$

In the 3-dim case applying the kinetic energy operator requires a 3-dim convolution with a filter that is a product of 3 1-dim filters. The operation count is $3 N_1 N_2 N_3 L$ where L is the length of the filter.

The nonlocal part of the pseudopotential

$$H^{sep}\Psi = |P\rangle\langle P|\Psi\rangle$$

where P is essentially a Gaussian in our case.

If the expansion coefficients c_J of P in a Daubechies wavelet/scaling function basis are known then

$$\begin{aligned}\langle P|\Psi\rangle &= \int \left(\sum_I c_I \phi(\mathbf{x} - I) \right) \left(\sum_J C_J \phi(\mathbf{x} - J) \right) d\mathbf{x} \\ &= \sum_J c_J C_J\end{aligned}$$

Because a Gaussian is separable and a 3-dim scaling function/wavelet basis is also a product of 1-dim scaling functions/wavelets the expansion coefficients $c_{i,j,k}$ can easily be calculated with machine precision.

$$\begin{aligned}c_{i,j,k} &= \int \int \int \phi_i^k(x) \phi_j^k(y) \phi_k^k(z) \exp(-(1/2)(x^2 + y^2 + z^2)) dx dy dz \\ &= \int \phi_i^k(x) \exp(-(x^2/2)) dx \int \phi_j^k(y) \exp(-(y^2/2)) dy \int \phi_k^k(z) \exp(-(z^2/2)) dz\end{aligned}$$

The potential energy

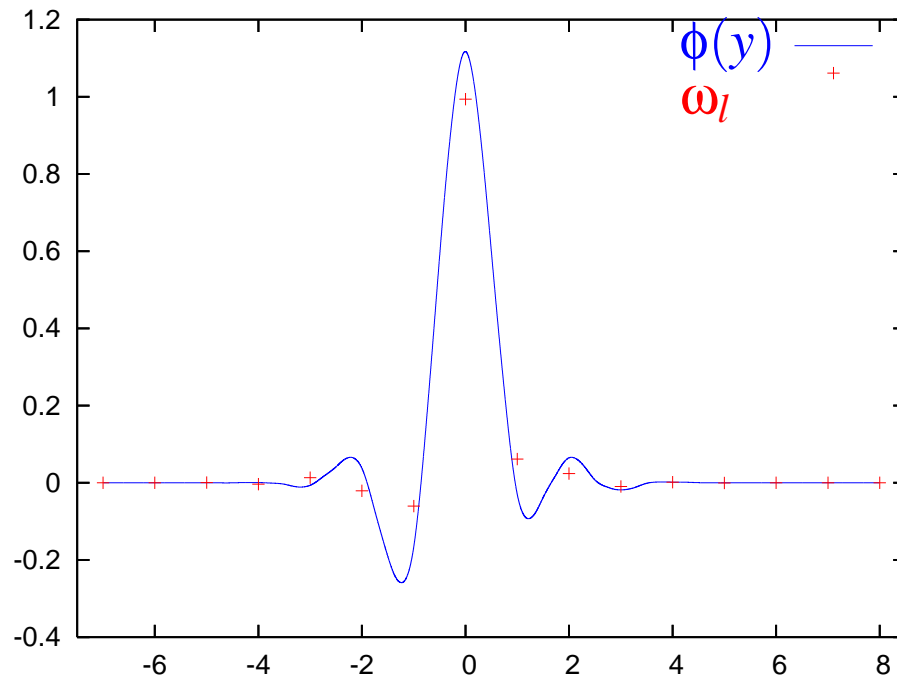
Problem: Daubechies are not smooth enough for conventional integration schemes.

The "magic filter" method

A. Neelov and S. Goedecker, J. of. Comp. Phys. 217, 312-339 (2006)

We do not calculate the values of Ψ on grid points, but we calculate the values $\bar{\Psi}_i$ that represent best Ψ in a neighborhood around the grid point

$$\bar{\Psi}_i = \sum_j \Psi_j \omega_{i-j} \quad ; \quad E_{pot} = \sum_i \bar{\Psi}_i V_i \bar{\Psi}_i$$



Convergence rates in BIGDFT

- potential energy convergence rate: h^{16}
- kinetic energy convergence rate: h^{14}
- total energy convergence rate: h^{14}
- convergence rate for error in wavefunctions: h^8
- error arising from magic filter approximation is much smaller than discretization error

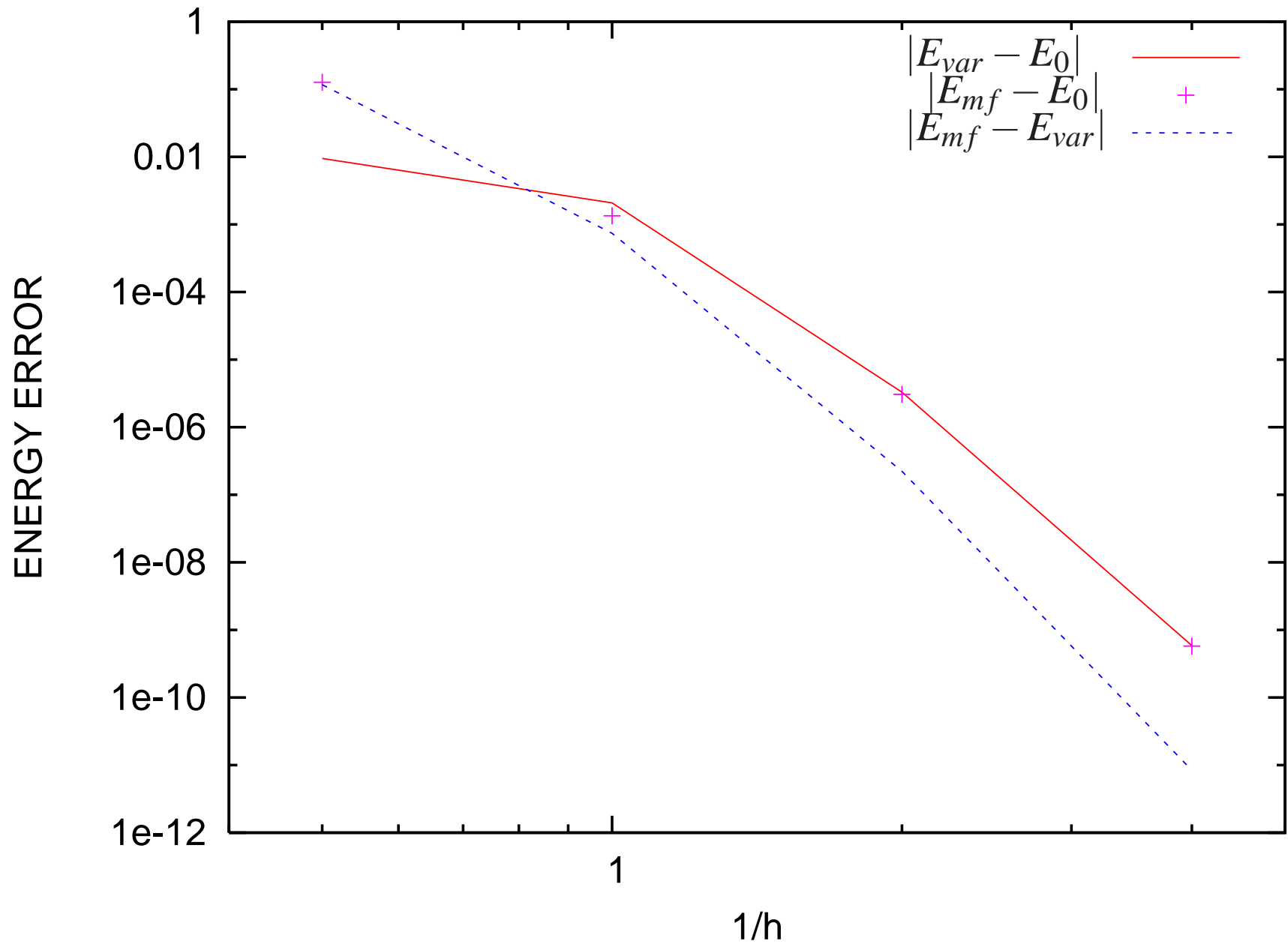


Figure 1: The result of energy minimization with the magic filter for the least asymmetric Daubechies-16 scaling functions.

Preconditioning

The preconditioning equation

$$\frac{1}{2}(\nabla^2 + C)\vec{p} = \vec{g}$$

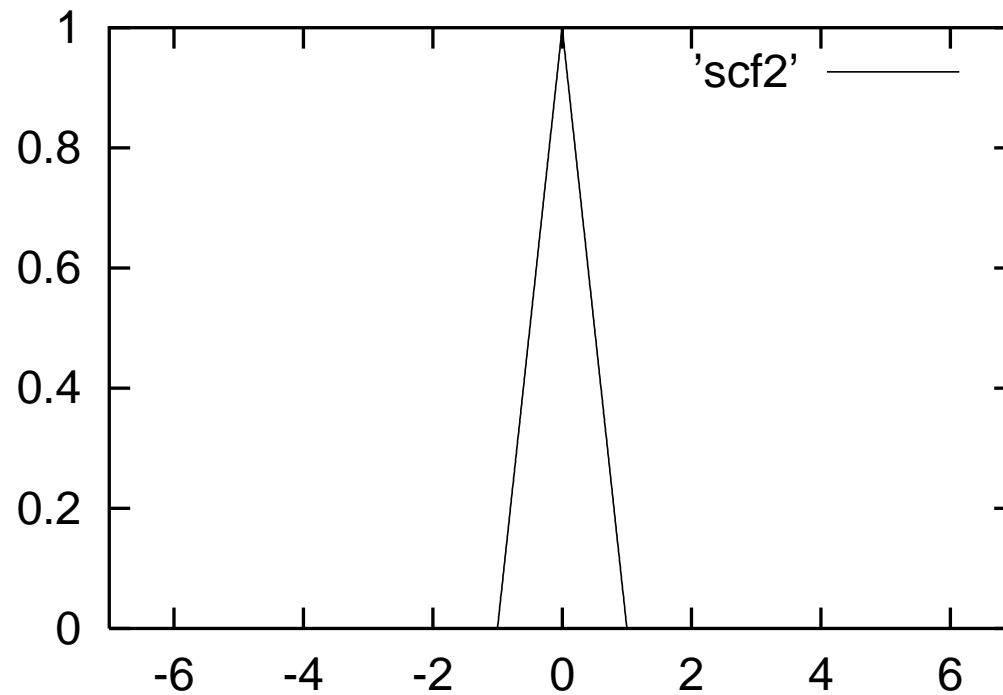
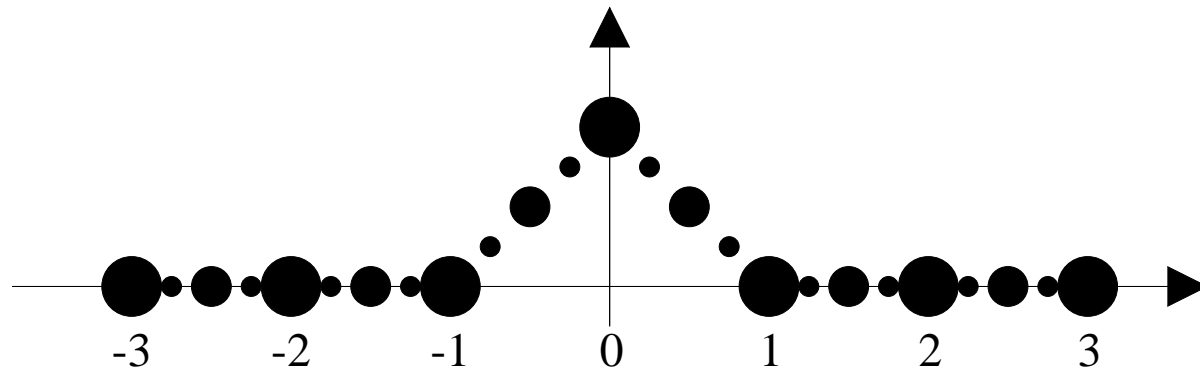
is solved iteratively by a multilevel preconditioned conjugate gradient method. 5 iterations are usually enough because Laplace operator is diagonally dominant in a wavelet basis.

Electronic charge density ρ is also obtained by magic filter

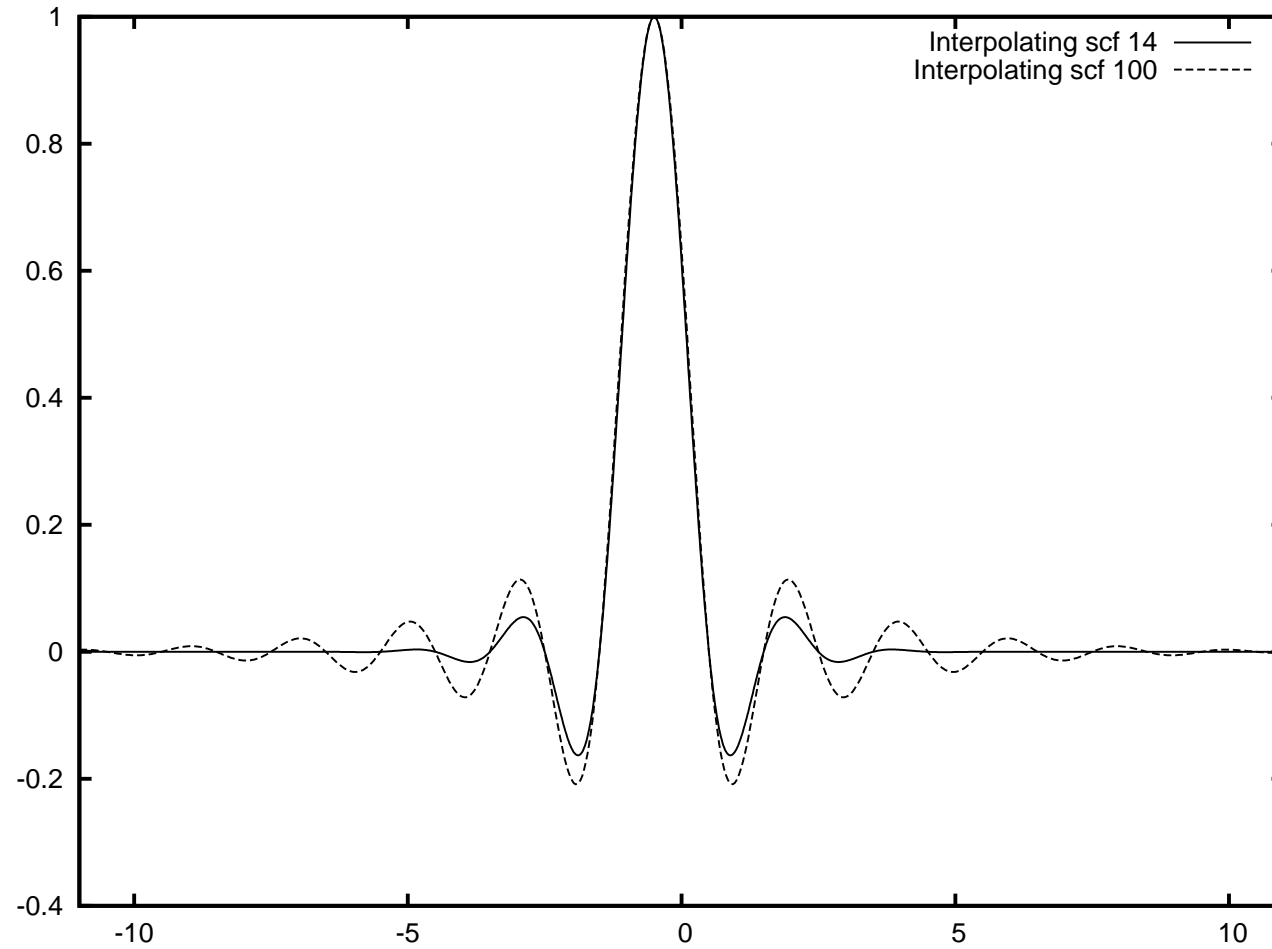
$$\rho_i = \bar{\Psi}_i \bar{\Psi}_i$$

Construction of interpolating scaling functions

Recursive interpolation from Kronecker data set: Example linear interpolation



High order interpolating scaling functions



Refinement relations:

$$\phi(x) = \sum_{j=-m}^m h_j \phi(2x - j)$$

Solution of Poisson's equation for free boundary conditions

L. Genovese, T. Deutsch, A. Neelov, S. Goedecker, G. Beylkin, J. Chem. Phys. 125 (2006)

Given the values of the charge density on a regular grid, $\rho_{i,j,k}$, the continuous charge distribution is represented in terms of interpolating scaling functions

$$\rho(\mathbf{r}) = \sum_{i,j,k} \rho_{i,j,k} \phi(x-i)\phi(y-j)\phi(z-k)$$

The moments of the discrete and continuous charge distributions $\rho_{i,j,k}$ and $\rho(\mathbf{r})$ are identical

$$\sum_{i,j,k} i^{l_1} j^{l_2} k^{l_3} \rho_{i,j,k} = \int d\mathbf{r} x^{l_1} y^{l_2} z^{l_3} \rho(\mathbf{r}) \quad (1)$$

if $l_1, l_2, l_3 < m$, where m is the order of the scaling functions. The potential at a grid point i_1, i_2, i_3 is given by

$$\begin{aligned} V_{i_1, i_2, i_3} &= \sum_{j_1, j_2, j_3} \rho_{j_1, j_2, j_3} \int \frac{\phi(x' - j_1)\phi(y' - j_2)\phi(z' - j_3)}{|r_{j_1, j_2, j_3} - r'|} dr' \\ &= \sum_{j_1, j_2, j_3} \rho_{j_1, j_2, j_3} K_{i_1 - j_1, i_2 - j_2, i_3 - j_3} \end{aligned}$$

The above convolution can be calculated rapidly with Fourier methods

The integral $K_{i-ip, j-jp, k-kp}$ becomes a sum of separable terms if $1/r$ is expanded in a sum of Gaussians

$$\frac{1}{r} \approx \sum_{k=1}^{89} \omega_k e^{-p_k r^2}$$

$$K_{j_1, j_2, j_3} = \sum_{k=1}^{89} \omega_k K_{j_1}(p_k) K_{j_2}(p_k) K_{j_3}(p_k)$$

We need to evaluate $89 \times \max(\{n_1, n_2, n_3\})$ integrals of the type

$$K_j(p) = \int \varphi_0(x) e^{-p(x-j)^2} dx$$

The efficiency in calculating the integrals can be improved using the refinement relation

$$\begin{aligned} K_i(4p) &= \int \varphi(x) e^{-4p(x-i)^2} dx \\ &= \frac{1}{2} \int \varphi(x/2) e^{-p(x-2i)^2} dx \\ &= \frac{1}{2} \sum_j h_j \int \varphi_j(x) e^{-p(x-2i)^2} dx \\ &= \frac{1}{2} \sum_j h_j K_{2i-j}(p) . \end{aligned}$$

In this way all the integrals can easily be calculated up to machine precision

Other wavelet codes

- Madness: All electron LDA code using a multi-wavelet basis
- code by T. Arias: DFT code using interpolating wavelets, development apparently abandoned

Summary

BigDFT

- uses Daubechies wavelets to represent the wavefunctions and interpolating scaling functions to represent the charge density
- is specifically tailored for large scale problems in nanosciences
- is already a high performance production code with all standard functionalities
- is under heavy further development