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Algorithm for the orthogonal fast discrete spherical Bessel transform on a uniform grid

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Motivation

- A pseudospectral method based on a fast Fourier transform (FFT) is widely used to solve partial differential equations. But this method is implemented only in Cartesian coordinates.
- Pseudospectral methods intended for spherical coordinates can be based on the spherical Bessel transform (SBT). But all the known algorithms for the SBT are inferior to the FFT in some aspects.
- Our goal was to create an algorithm for the spherical Bessel transform, which would have all the advantages of FFT.

Known algorithms

FFT	Convolution integral	SFB expansion on trigonometric funcs	Gauss-Bessel quadrature	SBF via Legendre polynomials
fast (N $\log_2$N ops.)	+	+	-	+
orthogonal	+	-	+	-
uniform grid	---	+	-	+

1) J.D. Talman, J. Comput. Phys. 29 (1978) 35.

2) O.A. Sharafeddin et al, J. Comput. Phys. 100 (1992) 294.

3) D. Lemoine, J. Chem. Phys. 101 (1994) 3936.

4) M. Toyoda, T. Ozaka, Comput. Phys. Comm. 181 (2010) 277.

Factorization of transformation

Spherical Bessel transformation (SBT): $$c_\ell(k) = \sqrt{\frac{2}{\pi}} \int_0^\infty \chi_\ell(kr)\psi_\ell(r)dr$$

Here $\chi_\ell(x) = xj_\ell(x)$, where $j_l(x)$ is a spherical Bessel function of l-th order (SBF)

$$j_\ell(z) = \frac{1}{2i^\ell} \int_{-1}^{1} P_\ell(\eta) \exp(iz\eta) d\eta$$

We can split the SBT into two successive steps:

1) Fourier transformation: $$\tilde{c}_\ell(k) = \sqrt{\frac{2}{\pi}} \frac{1}{2i^{\ell+1}} \int_0^\infty [e^{ikr} - (-1)^\ell e^{-ikr}]\psi_\ell(r)dr$$

2) Fourier-to Bessel transformation (FtB): $$c_\ell(k) = \tilde{c}_\ell(k) - \int_0^k \frac{P_\ell'(q/k)}{k} \tilde{c}_\ell(q)dq$$

Discretization

Radial grid: $r_i = (i - 1/2)\Delta r; \quad i = 1, \ldots, N.$

$$\psi_i = \psi_\ell(r_i)\sqrt{\Delta r}$$

Fourier transformation: $\mathbf{f} = \mathbf{F}\boldsymbol{\psi}$

$$f_n = \tilde{c}_\ell(k_n)\sqrt{w_n}$$

Transformation matrix:

$$F_{ni} = \sqrt{\frac{2 - \delta_{n0} - \delta_{nN}}{N}}(-1)^{\lceil \ell/2 \rceil} \times \begin{cases} \sin(k_n r_i), & \text{even } \ell; \\ \cos(k_n r_i), & \text{odd } \ell. \end{cases}$$

Momentum grid: $k_n = n\Delta k; \quad \begin{array}{ll} n = 1, \ldots, N & \text{even } \ell; \\ n = 0, \ldots, N-1 & \text{odd } \ell. \end{array}$

Fourier-to-Bessel transformation matrix

Integral kernel: $$T(k,q) = \delta(q-k) - \theta(k-q)\frac{P'_\ell(q/k)}{k}$$

Discrete FtB: $$\mathbf{b} = \mathbf{Tf}$$

Transformation matrix: $$T_{nm} = \alpha_n\left[\delta_{nm} - L_{nm}\right]$$

Lower-triangle matrix: $$L_{nm} = -\theta(n-m)P'_\ell(n-m,2n)\sqrt{1-\frac{\delta_{m0}}{2}}$$

Discrete “derivative” of DLOP: $$P'_\ell(i,N) = \frac{2}{1+P_\ell(-1,N-1)}\nabla[P_\ell](i,N-1)$$

Discrete Legendre orthogonal polynomials (DLOP)

Orthogonality condition: $$\sum_{i=0}^{N} P_\ell(i,N)P_\mu(i,N) = \mathcal{N}(\ell,N)\delta_{\ell\mu}$$

DLOP asymptotic form: $$P_\ell(i,N) = P_\ell(1-2i/N) + O(N^{-2})$$

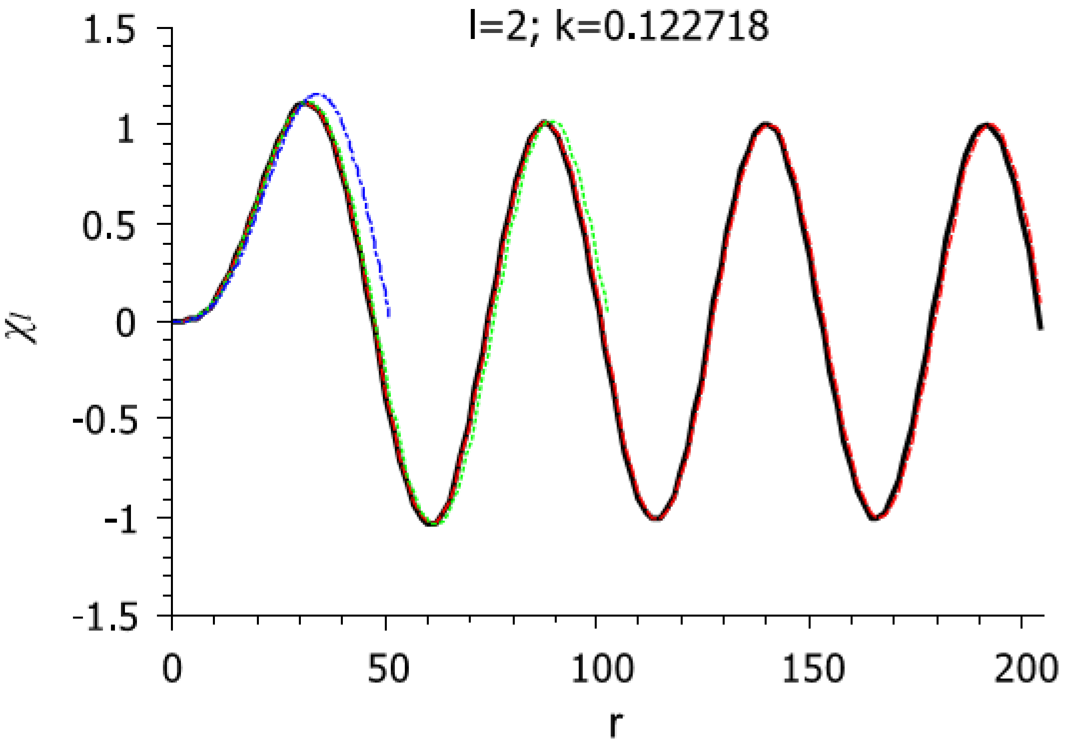
DDLOP satisfies condition $$\sum_{i=0}^{N} P'_\ell(i,N)p(i)w_i(N) = (-1)^\ell p(N) - p(0)$$

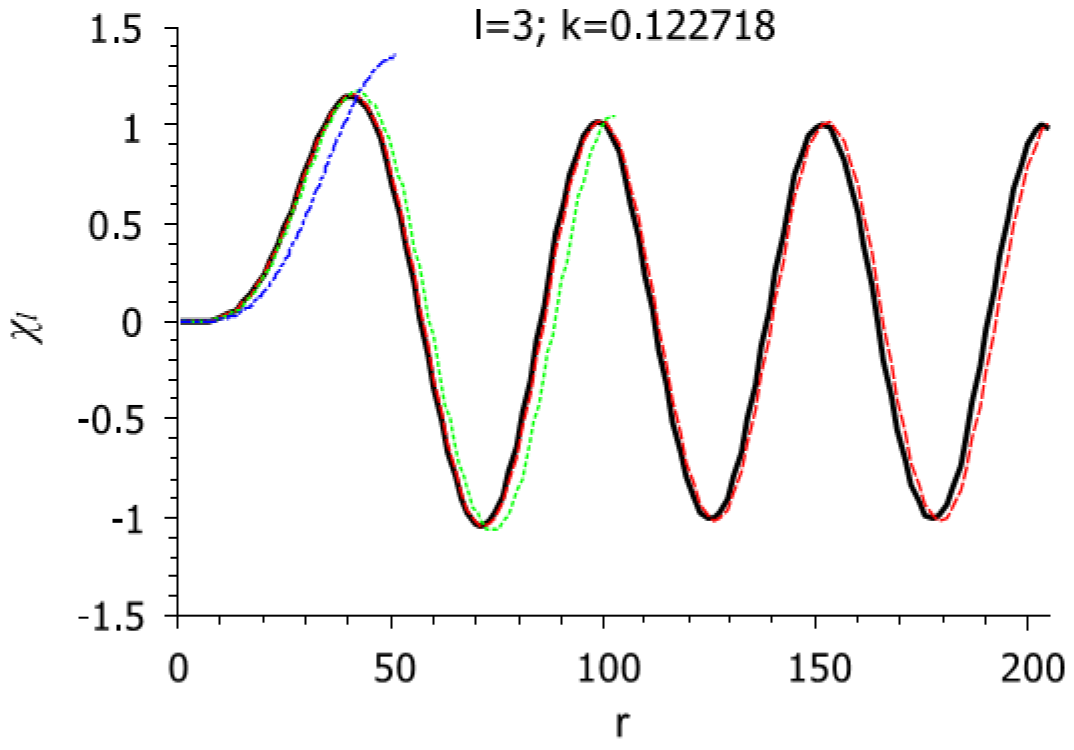
where *p*(*i*) is any polynomial of the degree $s \leq \ell$, and weight $w_i(N) = 1 - \dfrac{\delta_{iN} + \delta_{i0}}{2}$

DDLOP asymptotic form $$P'_\ell(i,N) = \frac{d}{di}P_\ell(1-2i/N) + O(N^{-3})$$

Accuracy

$$\tilde{\chi}_{n\ell}(r_i) = (r_{\max}/2)^{1/2} w_n^{-1/2} [\mathbf{F}^\dagger \mathbf{T}^T]_{i,n}$$





Error of present SBT method has the order $1/r_{\max}^2$ or Δk^2

Fast algorithm

By using of expansion

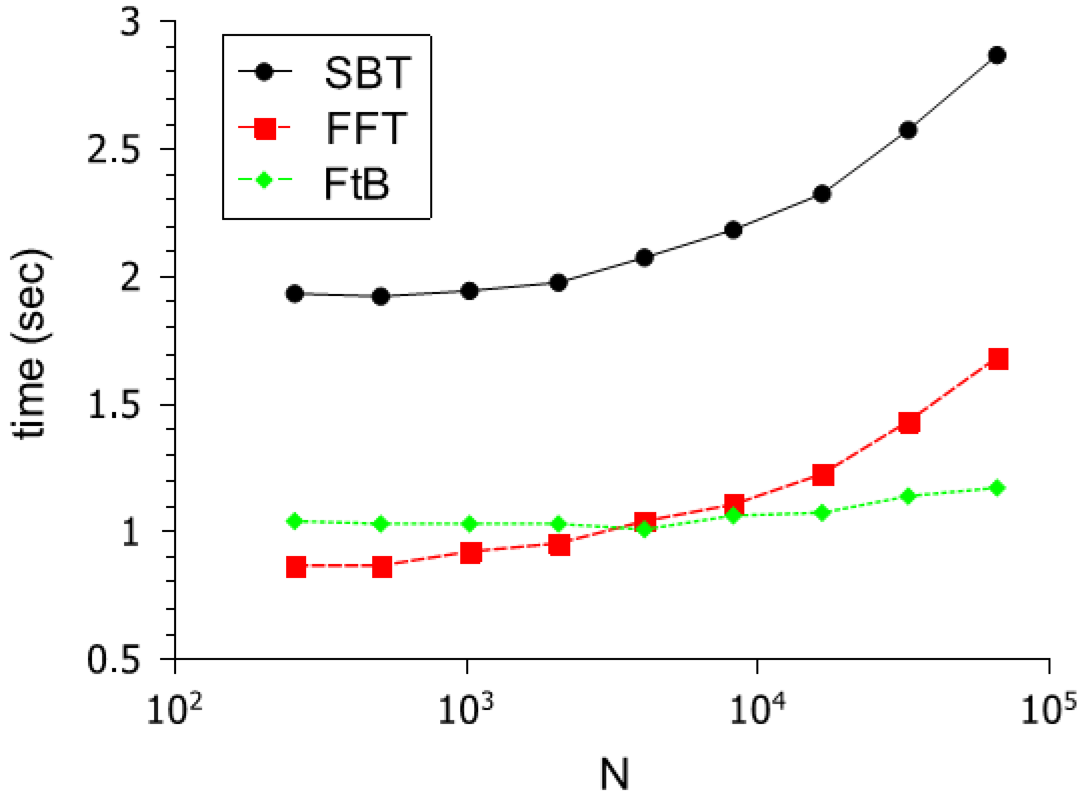
$$P'_\ell(n-m,2n) = -\sum_{\nu=0}^{\ell-1} \xi_{\ell\nu}(n) m^\nu .$$

we can write FtB as

$$b_n = \alpha_n f_n - \alpha_n \sum_{\nu=0}^{\ell-1} \xi_{\ell\nu}(n) s_{\nu n}$$

Recurrence relation

$$s_{\nu n} = s_{\nu,n-1} + \frac{1}{2}\left[n^\nu f_n + (n-1)^\nu f_{n-1}\right]$$



$\ell = 4$

Number of operations for FtB is lN + Number operation for FFT is $N \log_2 N$

Discrete Variable Representation (DVR)

Function in DVR in spherical coordinates: $\psi_{ijk} = \Psi(r_i, \arccos\eta_j, \phi_k) r_i \sqrt{\Delta r \Delta\eta_j \Delta\phi}$

Angular grid:
$\phi_k = \Delta\phi(k-1), \quad k = 1, \ldots, N_\phi$
η_j and $\Delta\eta_j, \quad j = 1, \ldots, N_\theta$ – nodes and weights of Gauss-Legendre quadrature

Transformation from DVR to spherical wave expansion: $\mathbf{c} = \mathbf{BY}\boldsymbol{\psi}$

SBT matrix: $B_{nlmil'm'} = [\mathbf{T}_l \mathbf{F}_l]_{ni} \delta_{ll'} \delta_{mm'}$

Angular transformation matrix: $Y_{ilmi'jk} = \delta_{ii'} [\mathbf{P}\boldsymbol{\Phi}]_{lmjk}$

$$P_{lmjm'} = \overline{P}_l^m(\eta_j)\sqrt{\Delta\eta_j}\,\delta_{mm'}$$

$$\Phi_{jmj'k} = \delta_{jj'} \frac{e^{im\phi_k}}{\sqrt{2\pi}} \sqrt{\Delta\phi}$$

Transformation from DVR to plane wave expansion: $\boldsymbol{\varphi} = \tilde{\mathbf{Y}}^\dagger \mathbf{BY}\boldsymbol{\psi}$

where $\tilde{Y}_{nlmn'jk} = \delta_{nn'} i^l [\mathbf{P}\boldsymbol{\Phi}]_{lmjk}$

Pseudospectral method for TDSE

$$i\frac{\partial \psi(r,\theta,\phi,t)}{\partial t} = \hat{H}\psi(r,\theta,\phi,t)$$

Hamiltonian:

$$\hat{H} = \frac{\hat{\vec{p}}^{\,2}}{2} - \vec{\mathscr{A}}(t)\hat{\vec{p}} + U(r,\theta,\phi,t)$$

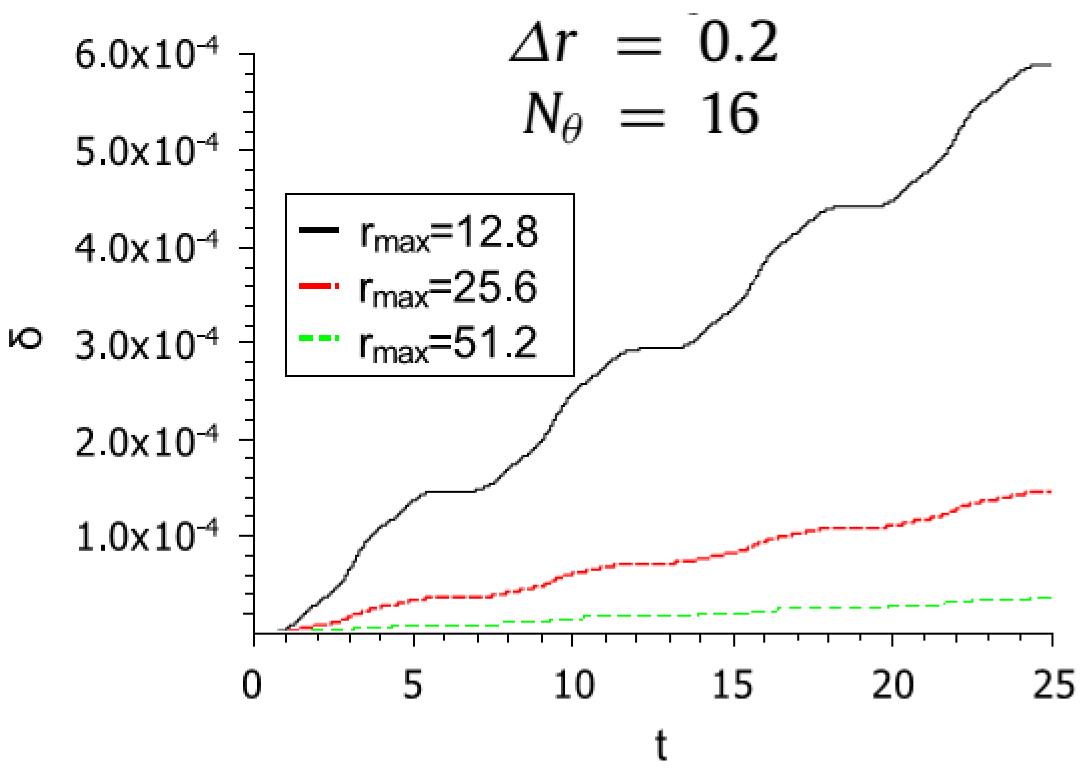
Hamiltonian matrix in DVR:

$$\mathbf{H}(t) = \mathbf{Y}^{\dagger}\mathbf{B}^{\dagger}[\mathbf{K} - \tilde{\mathbf{Y}}(\vec{\mathscr{A}}(t)\vec{\mathbf{P}})\tilde{\mathbf{Y}}^{\dagger}]\mathbf{B}\mathbf{Y} + \mathbf{U}(t)$$

$$\begin{aligned}
\boldsymbol{\psi}_1(t) &= \exp[-i\mathbf{U}(t+\tau/2)\tau/2]\boldsymbol{\psi}(t);\\
\mathbf{c}_1(t) &= \mathbf{B}\mathbf{Y}\boldsymbol{\psi}_1(t);\\
\mathbf{c}_2(t) &= \exp[-i\mathbf{K}\tau/2]\mathbf{c}_1(t);\\
\boldsymbol{\varphi}_2(t) &= \tilde{\mathbf{Y}}^{\dagger}\mathbf{c}_2(t);\\
\boldsymbol{\varphi}_3(t) &= \exp[i(\vec{\mathscr{A}}(t+\tau/2)\vec{\mathbf{P}})\tau]\boldsymbol{\varphi}_2(t);\\
\mathbf{c}_3(t) &= \tilde{\mathbf{Y}}\boldsymbol{\varphi}_3(t);\\
\mathbf{c}_4(t) &= \exp[-i\mathbf{K}\tau/2]\mathbf{c}_3(t);\\
\boldsymbol{\psi}_4(t) &= \mathbf{Y}^{\dagger}\mathbf{B}^{\dagger}\mathbf{c}_4(t);\\
\boldsymbol{\psi}(t+\tau) &= \exp[-i\mathbf{U}(t+\tau/2)\tau/2]\boldsymbol{\psi}_4(t).
\end{aligned}$$

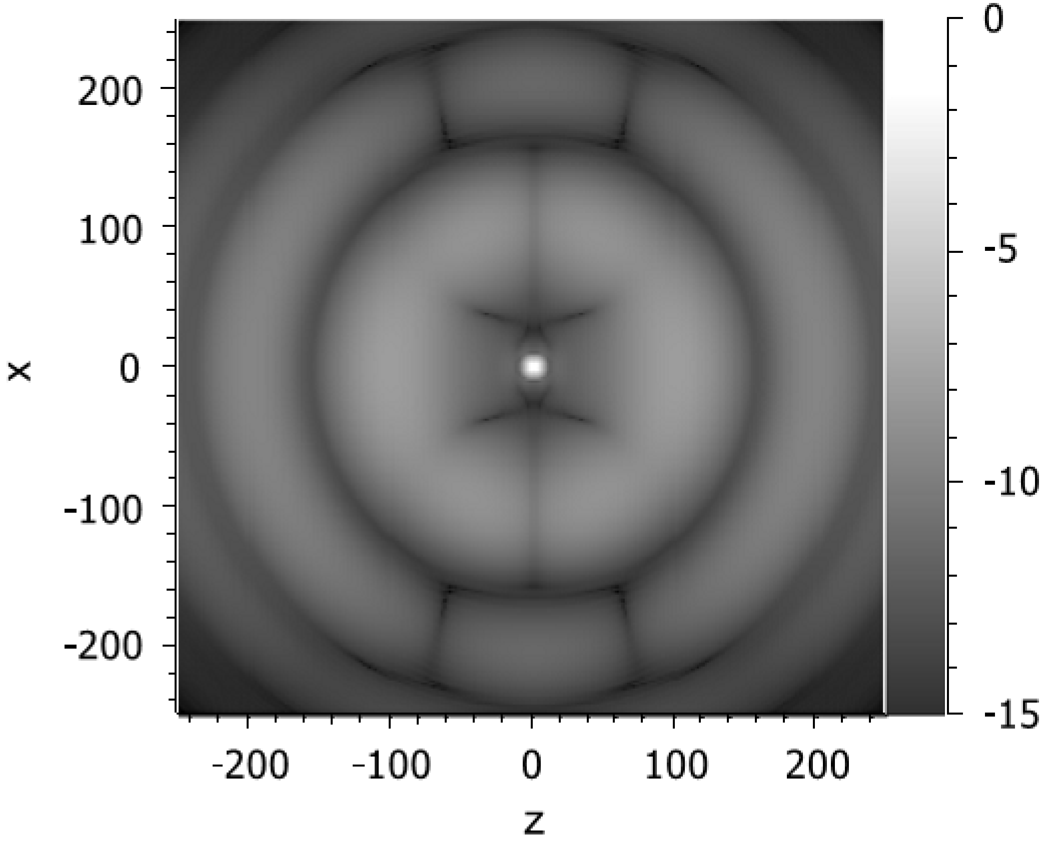
Tests and examples

Oscillator in external field



$$\delta(t) = |1 - \langle \psi_{osc}(\vec{r}, t) | \psi(\vec{r}, t) \rangle|$$

H_2^+ in external field



Electronic density as a function of (x,z)

Conclusion

- We developed the algorithm for the orthogonal fast discrete spherical Bessel transform on a uniform grid.
- Our approach is based upon the spherical Bessel transform factorization into the two subsequent orthogonal transforms, namely the fast Fourier transform and the orthogonal transform founded on the derivatives of the discrete Legendre orthogonal polynomials.
- The algorithm have applied for the numerical solution of the three-dimensional time-dependent Schrödinger equation.

See more details in the article:

Serov V. V. *Orthogonal fast spherical Bessel transform on uniform grid*
Computer Physics Communications **216** (2017) 63–76.

Thank you for attention!