Functional Decompositions and Algorithmic Basis Reduction in Multidimensional FEM Schemes

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Motivation: The Curse of Dimensionality

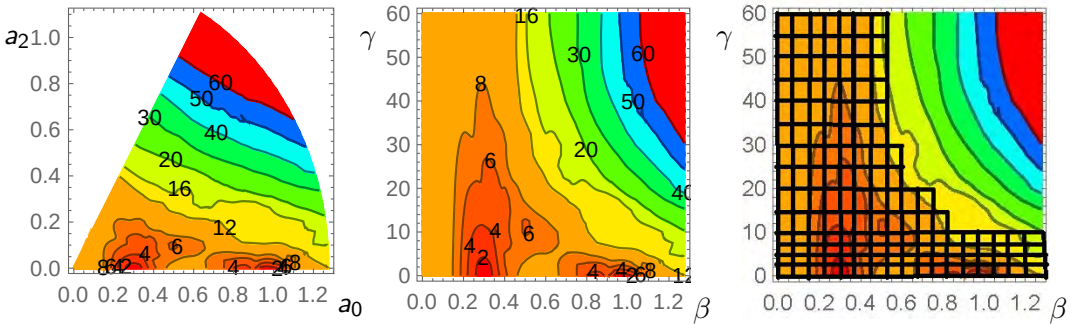
Physical Context

Modern calculations of vibrational-rotational spectra in **collective quadrupole-octupole models** of heavy atomic nuclei require solving systems of coupled elliptic PDEs.

The Bottleneck

- The configuration space is **6-dimensional**.
- Traditional Finite Difference Methods (FDM) and global Galerkin methods demand supercomputer resources.
- Researchers are often forced to limit calculations to 2D or 3D subdomains.

Our Goal: Develop efficient FEM schemes capable of solving 6D BVPs on **modern personal computers**.



Zhao, P. W., Li, Z. P., Yao, J. M., and Meng, J.: New parametrization for the nuclear covariant energy density functional with a point-coupling interaction, Phys. Rev. C 82, 054319–1–14 (2010).

Self-adjoint d-dimensional BVP for $\mathcal{N}$ coupled PDEs

$$\left(\mathbf{I}T(x) + \mathbf{Q}(x)\frac{\partial}{\partial x} + \frac{\partial}{\partial x}\mathbf{Q}(x) + \mathbf{V}(x) - E_v\mathbf{I}\right)\mathbf{\Phi}_v(x) = 0,$$

$$T(x) = -\frac{1}{g_0(x)}\sum_{i,j=1}^{d}\frac{\partial}{\partial x_i}g_{ij}(x)\frac{\partial}{\partial x_j}$$

$$\mathbf{Q}(x)\frac{\partial}{\partial x} + \frac{\partial}{\partial x}\mathbf{Q}(x) = \sum_{i=1}^{d}\frac{1}{g_0(x)}\mathbf{Q}^{(i)}(x)\frac{\partial}{\partial x_i} + \sum_{i=1}^{d}\frac{1}{g_0(x)}\frac{\partial}{\partial x_i}\mathbf{Q}^{(i)}(x)$$

Boundary Conditions

$$\mathbf{\Phi}_v(x)|_S = 0, \quad \frac{\partial\mathbf{\Phi}_v(x)}{\partial n_D}\Big|_S = 0, \quad \frac{\partial\mathbf{\Phi}_v(x)}{\partial n_D} = \sum_{ij=1}^{d}(\hat{n},\hat{e}_i)g_{ij}(x)\frac{\partial\mathbf{\Phi}_v(x)}{\partial x_j}.$$

The BVP is reduced to variation functional:

$$\int_\Omega \left(\sum_{ij=1}^{d} g_{ij} \frac{\partial \mathbf{\Phi}^T}{\partial x_i} \frac{\partial \mathbf{\Phi}}{\partial x_j} + g_0 \mathbf{\Phi}^T \mathbf{V} \mathbf{\Phi} + \sum_{i=1}^{d} \mathbf{\Phi}^T \mathbf{Q}^{(i)} \frac{\partial \mathbf{\Phi}}{\partial x_i} - \sum_{i=1}^{d} \frac{\partial \mathbf{\Phi}^T}{\partial x_i} \mathbf{Q}^{(i)} \mathbf{\Phi} - g_0 E \mathbf{\Phi}^T \mathbf{\Phi} \right) d^d x$$

The approximate solution is expanded over local basis functions $\mathbf{N}_{n(l)}(x)$:

$$\mathbf{\Phi}_v^h(x) = \sum_{l=1}^{L} \Phi_{l;v}^h \mathbf{N}_{n(l)}(x)$$

Multivariate Hermite Interpolation Polynomials (HIPs)

Key Feature: HIPs preserve the continuity of *derivatives* up to order κ_c across finite element boundaries.

- Crucial for correctly handling **mixed partial derivatives** in the PDEs.
- Ensure smooth FEM solutions on the boundaries of adjacent elements.
- Theoretical Error Estimates:
  Eigenvalues: $|E - E^h| \leq c_1 h^{2p}$
  Eigenfunctions: $\|\Phi - \Phi^h\|_0 \leq c_2 h^{p+1}$.

Algebraic Eigenvalue Problem & Basis Reduction

Generalized Algebraic Eigenvalue Problem

$$\left(\mathbf{A}^{(1)} + \mathbf{A}^{(2)} + \mathbf{A}^{(3)} - E_v^h \mathbf{B}\right) \mathbf{\Phi}_v^h = 0, \ \mathbf{\Phi}^T \mathbf{B} \mathbf{\Phi} = \mathbf{I}$$

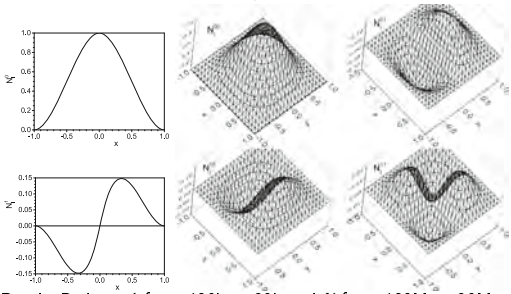
- $\mathbf{A}^{(i)}$ – stiffness matrices (symmetric)
- $\mathbf{B}$ – mass matrix (positive definite)
- Dimension: $L \times L$, where L is the number of basis functions
- Sparse structure with band-like pattern

Challenge: As dimension d increases:

- L grows exponentially, number of non-zero elements N grows even faster
- For $d = 6$: $L \sim 120$k, $N \sim 120$M without reduction

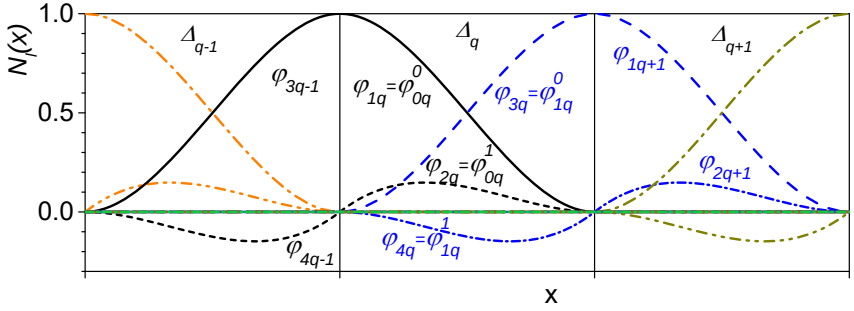
Algorithmic Basis Reduction

To restrain this growth, we exclude basis functions $N_l(x)$ for which the sum of orders of their higher mixed derivatives exceeds a threshold $\check{\kappa} : |\kappa_r| = \kappa_{r'_{i_1}1} + \ldots + \kappa_{r'_{i_d}d} \geq \check{\kappa}$



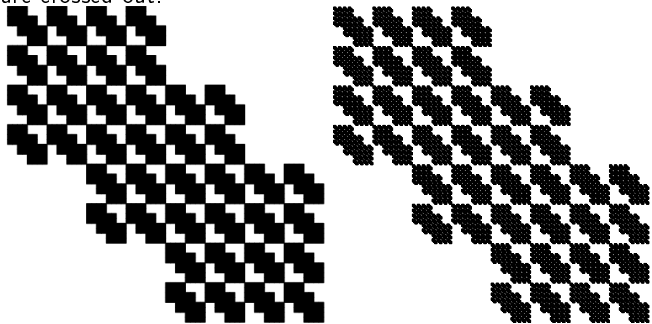
Result: Reduces L from 120k to 30k and N from 120M to 30M while preserving 3rd-order accuracy!

Basis of one-dimensional local functions



$$N_l(z) = \sum_{s'=0,1} \{\varphi_{r+ss',q-s'}(z), z \in \Delta_{q-s'}\}.$$

Due to the fact that each of the basis functions may not be equal to zero only on such regions Ω_q for which q_i may differ by no more than one and the approved ordering the complex self-similar structure of the matrices of the algebraic problems is followed. The example of structure of matrices for the d-dimensional problems $d = 2$ and $d = 3$ by the third order HIPs on square and cubic domains $q_i^{\max} = 3$, $i = 1, ..., d$ is presented in fig. When excluding basic functions or cells, the corresponding rows and columns are crossed out.



The Dirac oscillator equation produced by M. Moshinsky has the form:

$$\imath\frac{\partial\psi}{\partial x^0} = (\alpha\cdot(\mathbf{p}-\imath\omega\mathbf{r})+\beta)\psi,\ \psi = \begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}\exp(-\imath E x^0) \Rightarrow \begin{cases}(E-1)\psi_1 = (\sigma\cdot(\mathbf{p}+\imath\omega\mathbf{r}\beta)\psi_2,\\ (E+1)\psi_2 = (\sigma\cdot(\mathbf{p}-\imath\omega\mathbf{r}\beta)\psi_1\end{cases}$$

Multiplying the first equation by $(E+1)$ and using the second one we arrive that ψ_1 satisfies

$$(E^2-1)\psi_1 = (\mathbf{p}^2+\omega^2 r^2 - 3\omega - 4\omega\mathbf{L}\cdot\mathbf{S})\psi_1, \quad \mathbf{L} = \mathbf{r}\times\mathbf{p},\ \mathbf{S} = \frac{\sigma}{2}$$

The Dirac Oscillator in spherical coordinates

Coupled System for $\psi_1 = (\phi_1, \phi_2)^T$

$$\mathcal{L}\phi_1 + V_{11}\phi_1 + V_{12}\phi_2 + \frac{g_{22}}{g_{00}} Q_{12}^{\theta}\partial_\theta\phi_2 + \frac{1}{g_{00}}\partial_\theta(g_{22}Q_{12}^{\theta})\phi_2 = (E^2-1)\phi_1,$$

$$\mathcal{L}\phi_2 + V_{22}\phi_2 + V_{12}\phi_1 - \frac{g_{22}}{g_{00}} Q_{12}^{\theta}\partial_\theta\phi_1 - \frac{1}{g_{00}}\partial_\theta(g_{22}Q_{12}^{\theta})\phi_1 = (E^2-1)\phi_2,$$

where $\mathcal{L} = -\frac{1}{g_{00}}\left[\partial_r(g_{11}\partial_r) + \partial_\theta(g_{22}\partial_\theta)\right]$.

Metric & Potential Coefficients

$$g_{00} = r^2\sin\theta, \quad g_{11} = r^2\sin\theta, \quad g_{22} = \sin\theta,$$

$$V_{11} = \frac{m^2}{r^2\sin^2\theta} + \omega^2 r^2 - 2\omega m - 3\omega,$$

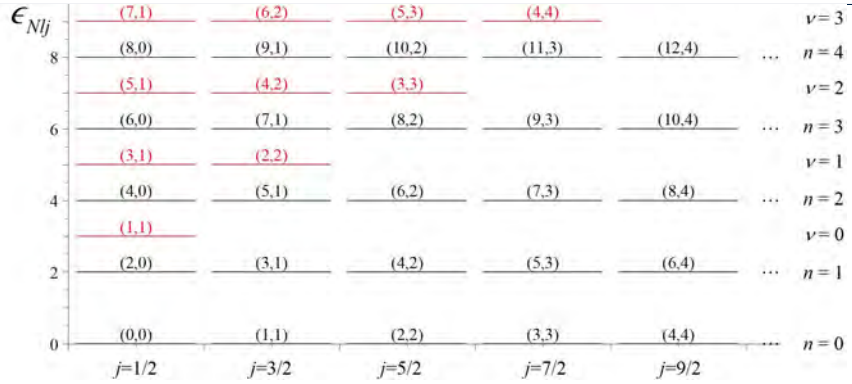
$$V_{12} = \omega(2m+1)\frac{\cos\theta}{\sin\theta},$$

$$V_{22} = \frac{(m+1)^2}{r^2\sin^2\theta} + \omega^2 r^2 + 2\omega(m+1) - 3\omega,$$

$$Q_{12}^{\theta} = \omega r^2.$$

Key features: Spin-orbit coupling via V_{12}, conormal derivatives on boundary, accidental degeneracy of spectrum.

Exact spectra of Dirac oscillator



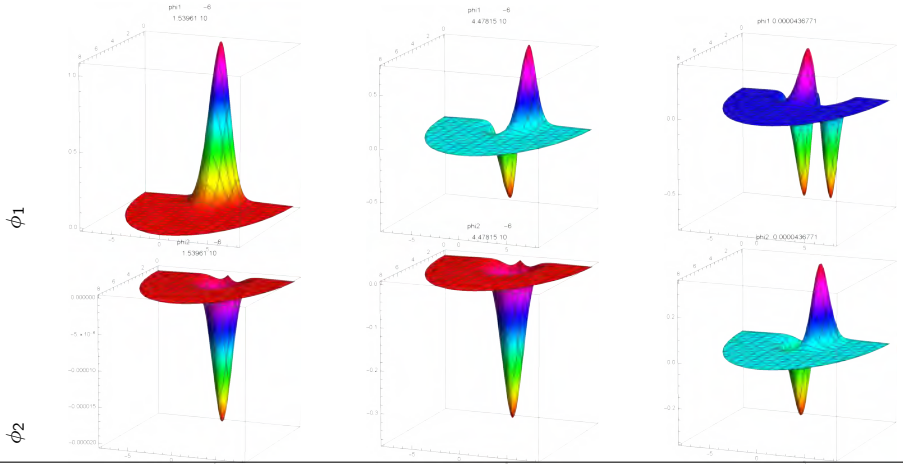
Energy spectrum ϵ_{Nlj} of the Dirac oscillator. The abscissa corresponds to the total angular momentum j and the ordinate $\epsilon_{Nlj} = \epsilon_\nu = (2\omega)^{-1}(E^2_{N,j+1/2,j} - 1) = 2\nu + 3$; $\nu = \frac{1}{2}(N + j - \frac{3}{2})$, $l = j + 1/2$, $\nu = 0, 1, 2...$ and $\epsilon_{Nlj} = \epsilon_n = (2\omega)^{-1}(E^2_{N,j-1/2,j} - 1) = 2n$; $n = \frac{1}{2}(N - j + \frac{1}{2})$, $\quad l = j - 1/2$, $n = 0, 1, 2....$ The values (N, l) are given above the levels.

The Dirac oscillator: Eigenfunctions

$E = 0,\ (N, L) = (0, 0)$ $E = 0,\ (N, L) = (1, 1)$ $E = 0,\ (N, L) = (2, 2)$

ϕ_1

ϕ_2

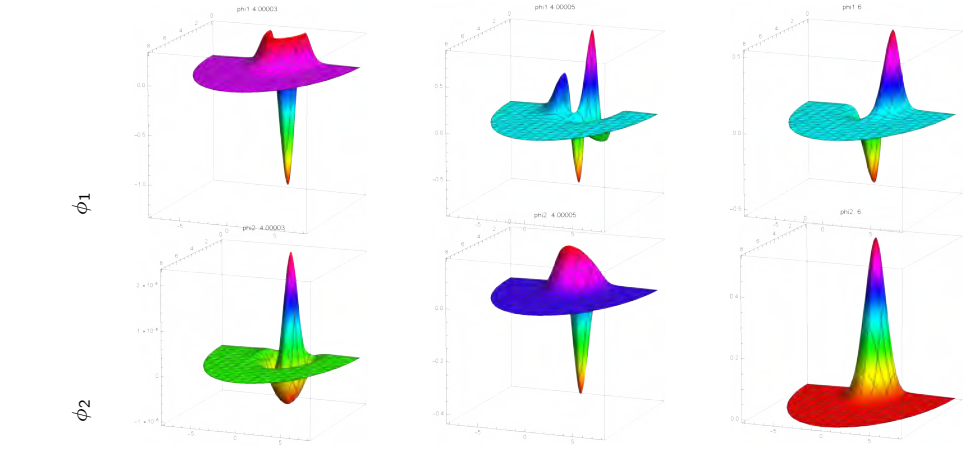


The Dirac oscillator: Eigenfunctions

$E = 4,\ (N, L) = (2, 0)$ $E = 4,\ (N, L) = (3, 1)$ $E = 6,\ (N, L) = (1, 1)$

ϕ_1

ϕ_2

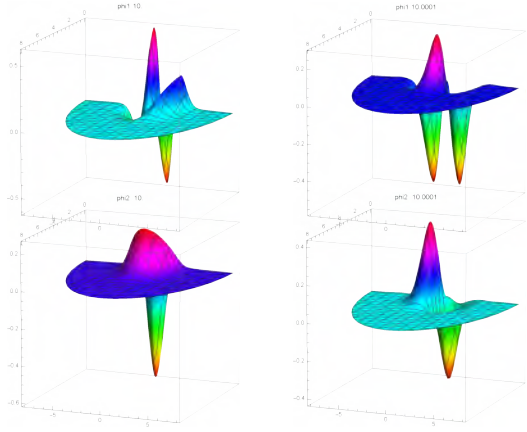


The Dirac oscillator: Eigenfunctions

$E = 10\,(N, L) = (3, 1)$ $E = 10\,(N, L) = (2, 2)$

ϕ_1

ϕ_2



Test 2: the Helmholtz problem on hyperellipsoid

$$\left(-\frac{1}{g_0(x)}\sum_{i,j=1}^{2}\frac{\partial}{\partial x_i}g_{ij}(x)\frac{\partial}{\partial x_j}-\frac{\partial^2}{\partial z^2}-E_v\right)\Psi_v(\theta_1,r,z)=0,$$

$$\Omega_3(x,z)=\left\{(\theta_1,r,z)\in\mathbb{R}^3\middle|0\le\theta_1<2\pi, r^2+\frac{z^2}{a_3^2}<1\right\},$$

$$x_1=a_1 r\sin\theta_1,\quad x_2=a_2 r\cos\theta_1,\quad x_3=z,$$

$x=(x_1,x_2)$, $x_1\equiv\theta_1$, $x_2\equiv r$.

$$g_0(x)=r,\quad g_{11}(x)=r^{-1}(\cos^2\theta_1/a_1^2+\sin^2\theta_1/a_2^2),$$
$$g_{12}(x)=g_{21}(\theta_1,r)=(1/a_1^2-1/a_2^2)\sin\theta_1\cos\theta_1,$$
$$g_{22}(x)=r(\sin^2\theta_1/a_1^2+\cos^2\theta_1/a_2^2).$$

Test 2: the Helmholtz problem on hyperellipsoid

We seek a solution $\Psi_v(x,z)$ using the two-dimensional KM in the form of an expansion in basis functions $B_n(z;x)$ with unknown coefficient functions $\Phi_{nv}(x)$.

$$\Psi_v(x,z) = \sum_{n=1}^{\mathcal{N}} B_n(z;x)\mathbf{\Phi}_{nv}(x).$$

Two-parameter basis functions $B_n(x;z) \equiv B_n(z;\theta_1,r)$ of the independent variable z on the interval $z \in (z_{\min}, z_{\max})$, where $z_{\min} = -a_d\sqrt{1-r^2}$, $z_{\max} = a_d\sqrt{1-r^2}$ and the corresponding eigenvalues $E_n(x)$ are known in analytical form and depend only on the parameter $x_2 = r$:

$$B_n(z;x) = \frac{\sin\left(\frac{(z+a_d\sqrt{1-r^2})\pi n}{2a_d\sqrt{1-r^2}}\right)}{\sqrt{a_d\sqrt{1-r^2}}}, \quad E_n(x) = \frac{\pi^2 n^2}{4a_d^2(1-r^2)}.$$

Test 2: the Helmholtz problem on hyperellipsoid

Integrated over $B_n(z,x)$ by $z \in (z_{\min}, z_{\max})$ with the orthogonality of the basis functions taken into account, we arrive at a system of PDEs in the domain $\Omega_2(x) \subset \mathbb{R}^2$, where the matrix elements at $d = 3$ and $a_0 = 1$ are given by formulas

$$Q^{(i)}_{n'n}(x) = g_{d-1i}(x)\frac{n'n(1+\cos(\pi n')\cos(\pi n))}{(n^2-n'^2)}\frac{r}{(a_0^2-r^2)}, \quad i = 1,2,$$

$$H_{n'n}(x) = \frac{g_{d-1d-1}(x)}{g_0(x)}\frac{2n'n(n^2+n'^2)(1+\cos(\pi n')\cos(\pi n))}{(n^2-n'^2)^2}\frac{r^2}{(a_0^2-r^2)^2},$$

$$H_{nn}(\theta_1, r) = \frac{g_{d-1d-1}(x)}{g_0(x)}\frac{\pi^2 n^2+3}{12}\frac{r^2}{(a_0^2-r^2)^2},$$

$$V_{nn'}(x) = E_n(x)\delta_{nn'} + H_{nn'}(x) + U_{nn'}(x), \quad U_{nn'}(x) = 0, \quad Q^{(i)}_{nn}(x) = 0.$$

The eigenfunctions $\mathbf{\Phi}_v(x_1,x_2) = (\Phi_{1v}(x_1,x_2), \Phi_{2v}(x_1,x_2), ...\Phi_{\mathcal{N}v}(x_1,x_2))^T$ of the discrete spectrum E: $E_1 \le E_2 \le ... \le E_v \le ...$ obey the BCsconsidering the above symmetries of the problem.

Test 2: the Helmholtz problem on hyperellipsoid

Symmetry Reduction

Exploit spatial symmetries to solve the BVP in a reduced subdomain $\Omega_2' = (0, \frac{\pi}{2}) \times (0, 1)$ (**1/4** of the full domain).

Solutions are classified by parity indices $t_i \in \{e, o\}$ (even/odd w.r.t. $x_i = 0$).

Boundary Conditions

- **Outer boundary** ($r = 1$): Dirichlet ($\Phi = 0$)
- **Origin** ($r = 0$): Regularity condition
- **Symmetry planes** ($\theta_1 = 0, \frac{\pi}{2}$):
  - Odd parity (o): Dirichlet ($\Phi = 0$)
  - Even parity (e): Neumann ($\frac{\partial \Phi}{\partial n} = 0$)

Explicit BCs for $\Phi \equiv \Phi_{nv}^{t_1 t_2 t_3}$

$$\Phi(\theta_1, 1) = 0,$$

$$r \frac{\partial \Phi}{\partial r}\bigg|_{r=0} = 0 \quad \text{or} \quad \Phi|_{r=0} = 0,$$

At $\theta_1 = 0$:

$$\Phi = 0 \ \ (t_1{=}o) \ \text{ or } \ \frac{\partial \Phi}{\partial \theta_1} = 0 \ \ (t_1{=}e),$$

At $\theta_1 = \frac{\pi}{2}$:

$$\Phi = 0 \ \ (t_3{=}o) \ \text{ or } \ \frac{\partial \Phi}{\partial \theta_1} = 0 \ \ (t_3{=}e).$$

Test 2: Helmholtz Problem (Cylindrical Symmetry)

Symmetry & Angular Dependence

For an oblate/prolate spheroid ($a_1 = a_2 \neq a_3$), eigenfunctions are characterized by **z-parity** $\sigma = \pm 1$ and magnetic quantum number $m = 0, 1, 2, \ldots$:

$$\Phi_v^{m,\sigma}(r, \theta_1, z) \propto \Phi_n^{m,\sigma}(r, z) \times \begin{cases} \cos(m\theta_1) \\ \sin(m\theta_1) \end{cases}$$

Mapping of symmetry indices $t_i \in \{e, o\}$ to m:

- $t_1 t_2 t_3 = \{ee*, oo*\} \implies m = 0, 2, 4, \ldots$ *(even)*
- $t_1 t_2 t_3 = \{eo*, oe*\} \implies m = 1, 3, 5, \ldots$ *(odd)*

Computational Setup

- **System:** $\mathcal{N} = 28$ coupled PDEs
- **Mesh:** $\{0 \ldots \pi/2\} \times \{0 \ldots 1\}$
- **Basis:** 4th-order HIPs
- **Code:** `GCMFEM9` (Mathematica)

Results

- Eigenvalues $E_v^{t_1 t_2 t_3}$ calculated
- Accuracy: **4 significant digits** vs etalon.
- Cross-validation with Fortran code `GCMFEM8`: $\Delta E \sim 10^{-3}$.

Test 2: Helmholtz Problem ($\sigma = +1$)

Lower part of the spectrum $E_\nu^{t_1 t_2 t_3}$ for 3D ellipsoids

E_ν^{eee}	E_ν^{eoe}, E_ν^{oee}	E_ν^{eee}, E_ν^{ooe}	E_ν^{eoe}, E_ν^{oee}	E_ν^{eee}, E_ν^{ooe}	E_ν^{eoe}, E_ν^{oee}	
ν	$m = 0$	$m = 1$	$m = 2$	$m = 3$	$m = 4$	$m = 5$
1	11.229170984	21.84594348	35.1501001	51.029602	69.410248	90.23847
	11.2292	21.8461	35.150	51.030	69.411	90.240
2	37.7674466	55.878366	76.100923	98.47922		
	37.768	55.879	76.10	98.48		
3	47.5391890	66.871385	89.39125			
	47.539	66.872	89.392			
4	77.969986					
	77.97					
5	92.39580					
	92.40					

Top row: GCMFEM8 (Fortran, etalon). **Bottom row:** GCMFEM9 (Mathematica).

Test 2: Helmholtz Problem ($\sigma = -1$)

Lower part of the spectrum $E_v^{t_1 t_2 t_3}$ for 3D ellipsoids

	E_v^{eeo}	E_v^{eoo}, E_v^{oeo}	E_v^{eee}, E_v^{ooo}	E_v^{eoo}, E_v^{oeo}	E_v^{eee}, E_v^{ooo}
v	$m = 0$	$m = 1$	$m = 2$	$m = 3$	$m = 4$
1	25.19769176	39.0583771	55.470743	74.367498	95.69921
	25.198	39.058	55.471	74.368	95.700
2	57.311351	77.907026			
	57.31	77.91			
3	76.263879	99.50419			
	76.264	99.50			

Top row: GCMFEM8 (Fortran, etalon). **Bottom row:** GCMFEM9 (Mathematica)

The dimension of the algebraic problem L, the number of nonzero elements N ($\times 10^6$), the CPU time T (min:sec), and the maximum memory M (Gb) , and the first five eigenvalues $E_i^{e\ldots e}$ of states symmetric with respect to $\hat{x}_i = 0$, $i = 1, ..., d$. The calculations was performed on grid $\Omega_{\theta_1,\ldots,\theta_{d-1},r} = \{0(h_{\theta_1} = \pi/6)\pi/2\}^{d-1} \otimes \{0(h_r = 1/4)1\}$. The lines marked by K represent the spectrum obtained by KANTBP for each d.

p	κ_r^c	$\check{\kappa}$	L	N	T	M	$E_1^{e\ldots e}$	$E_2^{e\ldots e}$	$E_3^{e\ldots e}$	$E_4^{e\ldots e}$	$E_5^{e\ldots e}$
$d = 4$											
2	0		2744	0.22	0:01	0.03	16.19474	42.87042	42.87089	46.70737	57.08947
3	1	2	1344	0.13	0:01	0.02	16.19242	42.88711	42.91700	46.66289	56.83628
3	1	3	3072	0.66	0:07	0.08	16.19229	42.77429	42.77490	46.56052	56.80268
3	1	4	4288	1.26	0:13	0.15	16.19229	42.77423	42.77425	46.56028	56.80261
3	1		4608	1.44	0:17	0.17	16.19229	42.77423	42.77425	46.56028	56.80261
3	0		12000	2.63	0:23	0.29	16.19229	42.77380	42.77384	46.55939	56.80067
	K						16.19229	42.77323	42.77323	46.55839	56.79836

p	κ_r^c	$\check{\kappa}$	L	N	T	M	$E_1^{e\ldots e}$	$E_2^{e\ldots e}$	$E_3^{e\ldots e}$	$E_4^{e\ldots e}$	$E_5^{e\ldots e}$
$d = 5$											
2	0		19208	5.48	2:55	1.25	21.84884	51.15097	51.15147	51.15294	56.08100
3	1	2	6400	1.87	1:24	0.31	21.84620	51.18729	51.19003	51.22003	56.03220
3	1	3	17664	13.73	10:02	2.12	21.84599	51.03087	51.03116	51.03194	55.88135
3	1	4	29440	37.28	32:21	5.53	21.84599	51.03077	51.03079	51.03081	55.88072
3	1	5	35584	53.84	42:17	8.35	21.84599	51.03077	51.03079	51.03081	55.88071
3	1		36864	57.62	76:17	8.35	21.84599	51.03077	51.03079	51.03081	55.88071
3	0		120000	120.95							
	K						21.84596	51.02965	51.02965	51.02965	55.87842
$d = 6$											
2	0		134192								
3	1	2	29624	25.17	101:47	5.97	28.17052	60.08334	60.12071	60.12652	60.14350
3	1	3	95328	225.23							
	K						28.17032	59.91105	59.91105	59.91105	59.91105

Conclusion

Key Achievements

- **Method:** Developed FEM schemes with Multivariate HIPs and **Algorithmic Basis Reduction** to overcome the exponential growth of matrix elements in high dimensions.
- **Computational Efficiency:** The reduction algorithm allows solving large Algebraic Eigenvalue Problems (AEP) on standard hardware:
  - **Current Capability:** $L \sim 30,000$, Non-zeros ~ 20M. $\implies$ High accuracy for 2D–4D; feasible for 5D–6D.
  - **Target (6D):** $L \sim 70,000$, Non-zeros ~ 70M.

Main Practical Impact

Six-dimensional BVPs for calculating spectra of quadrupole-octupole collective nuclear models are now solvable on modern personal computers (e.g., Intel Core i7, 16 GB RAM), eliminating the need for supercomputers.