Tensor-Structured Numerical Methods
for Solving Multidimensional Equations

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1. Motivating applications:

Modelling of large molecular systems such as proteins, bio-molecules and nanostructures. Molecular dynamics. Computational problems in financial math., machine learning, stochastic PDEs, multiparametric optimization, etc.

2. Main computational difficulties:

Exponential scaling in dimension for traditional \( O(n^d) \)-methods of linear complexity, "curse of dimensionality".

3. Novel Approach:

Tensor-structured numerical methods for representation of \( d \)-variate functions, operators and for solving physical equations in \( \mathbb{R}^d \), all with linear \( O(dn) \)-scaling in dimension \( d \),

\[
\mathbb{R}^{n^d} \leftrightarrow \mathbb{R}^n \otimes \ldots \otimes \mathbb{R}^n, \quad \mathbb{R}^{m^d \times n^d} \leftrightarrow \mathbb{R}^{mn} \otimes \ldots \otimes \mathbb{R}^{mn}.
\]
Linear/nonlinear spectral/b.v. problems in $\mathbb{R}^d$:

- Compute a pair $(\lambda, u) \in \mathbb{R} \times H^1_0(\Omega)$, s.t., $\langle u, u \rangle = 1$,

$$\Lambda u := -\text{div}(A \text{grad } u) + Vu = \lambda u \quad \text{in} \quad \Omega,$$

$$u = 0 \quad \text{on} \quad \partial \Omega.$$

- BVPs: Find $u \in H^1_0(\Omega)$, s.t.,

$$\Lambda u = F \quad \text{in} \quad \Omega.$$

Specific features:

- High spacial dimension: $\Omega = (-b, b)^d \in \mathbb{R}^d \ (d = 2, 3, ..., 100, ...)$.  
- Multiparametric equations: $A(x, a), V(x, a), a \in \mathbb{R}^M \ (M = 1, 2, ..., 100)$.  
- Nonlocal (integral) operator $V$, singular potentials.  
- Nonlinear operator $V$.  

1929, Dirac:

The fundamental laws necessary for the mathematical treatment of large part of physics and the whole of chemistry are thus completely known, and the difficulty lies only in the fact that application of these laws leads to equations that are too complex to be solved.

1998, W. Kohn, A. Pople:

Nobel Prize in Chemistry for development of DFT, based on computations via (separable) GTO basis sets.

Nowadays: Development of numerical tensor methods in multi-dimensional modeling that includes:

– Effective nonlinear approximation of operators and functions in $\mathbb{R}^d$,
– tensor-structured iterative methods,
– optimistic numerics in computational chemistry, sPDEs, NMLA,
– attempts to understanding the deep math. behind.
The Hartree-Fock equation,

$$\left[ -\frac{1}{2}\Delta - V(x) + \int_{\mathbb{R}^3} \frac{\rho(y)}{||x-y||} dy \right] \phi_i(x) - \frac{1}{2} \int_{\mathbb{R}^3} \frac{\tau(x, y)}{||x-y||} \phi_i(y) dy = \lambda \phi_i(x)$$

with $\phi_i \in H^1(\mathbb{R}^3)$,

$$\int_{\mathbb{R}^3} \phi_i \phi_j = \delta_{ij}, 1 \leq i, j \leq N_e,$$ where

$$\tau(x, y) = \sum_{i=1}^{N_e} \phi_i(x) \phi_i(y)$$ - electron density matrix,

$$\rho(x) = \tau(x, x)$$ - electron density,

$$\frac{1}{||x||}$$ - Newton potential,

$$V(x)$$ - Coulomb potential with singularities at the nuclei.
Def. 1. (Canonical format) Class of tensors in 
\( \mathbb{V}_n := H_1 \otimes \ldots \otimes H_d, \ H_\ell = \mathbb{R}^n \), that allow \( R \)-term representation

\[
\mathcal{C}_R = \left\{ w \in \mathbb{H} : w = \sum_{k=1}^{R} w_k^{(1)} \otimes w_k^{(2)} \otimes \ldots \otimes w_k^{(d)}, \ w_k^{(\ell)} \in H_\ell \right\}.
\]

\( w \in \mathcal{C}_R \) with \( w \notin \mathcal{C}_{R-1} \), has the tensor rank \( R \).

**Advantage:**

Tremendous reduction of the computational cost,

\( n^d \rightarrow d R n \) (linear in \( d \)).

**Limitations:**

Nonstable computation of the nearly optimal rank-\( R \) approximations, no directional adaptivity, lack of theory.
Choose $V_\ell \subset H_\ell$, with an orthonormal basis \( \{ \phi_{k,\ell} : 1 \leq k \leq r_\ell \} \),

\[ r_\ell := \text{dim } V_\ell \ll n \ (1 \leq \ell \leq d), \text{ i.e., } T^{(\ell)} = [\phi_1^{(\ell)} ... \phi_{r_\ell}^{(\ell)}] \in S_{r_\ell} \]

– the Stiefel manifold of the orthogonal $n \times r_\ell$ matrices.

\[ \mathbb{V}(r) = V_1 \otimes V_2 \otimes \ldots \otimes V_d \subset \mathbb{H} \equiv \mathbb{V}_n. \]

\[ v = \sum_{k=1}^r b_k \phi_{k_1}^{(1)} \otimes \phi_{k_2}^{(2)} \otimes \ldots \otimes \phi_{k_d}^{(d)} \in \mathbb{V}(r), \quad r = (r_1, \ldots, r_d), \]

\[ k = (k_1, \ldots, k_d), \ 1 \leq k_\ell \leq r_\ell, \ 1 \leq \ell \leq d, \text{ core tensor } \beta = [b_k]. \]

**Def 2. (Tucker format)** Given $r$, define \( T_{r,n} \subset \bigcup_{S_{r_\ell}} \mathbb{V}(r), \)

\[ T_{r,n} = \left\{ v \in \mathbb{V}_n : v = \beta \times_1 T^{(1)} \times_2 T^{(2)} \ldots \times_d T^{(d)}, \ b_k \in \mathbb{R} \right\}. \]

Storage: \( r^d + rdn \ll n^d, \ r = \max_\ell r_\ell \ll n, \ (r = O(\log n)). \)
Def. 3. (Two-level Tucker-canonical model), $\mathcal{T}_{C_{R,r}}$.

Subclass $\mathcal{T}_{C_{R,r}} \subset \mathcal{T}_{r,n}$ with $\beta \in C_{R,r} \subset V_r$,

$$v = \left( \sum_{\nu=1}^{R} \beta_{\nu} u_{\nu}^{(1)} \otimes \ldots \otimes u_{\nu}^{(d)} \right) \times_1 T^{(1)} \times_2 T^{(2)} \ldots \times_d T^{(d)}.$$

Storage: $dRr + R + drn$ (linear scaling in $d, n, R, r$).

[BNK '06]

Level I: Tucker decomposition (left). Level II: canonical decomposition of $\beta$ (right).
Problem 1. Best rank-$R$ approximation of $f \in \mathbb{V}_n$ in $\mathcal{C}_R$.

Problem 2. Best rank-$r$ orthogonal approx. of $f \in \mathbb{V}_n$ in $\mathcal{T}_r$.

Problem 3. Best rank-$(R, r)$ two-level orthogonal approximation of a high-order tensor $f \in \mathbb{V}_n$ in the set $\mathcal{T}_{\mathcal{C}_R, r}$.

$\mathcal{T}_r$ and $\mathcal{C}_R$ are not linear spaces $\Rightarrow$ a nontrivial nonlinear approximation problem.

Def. 4. (Tensor truncation $T_S : S_1 \to S$).

Given $A \in S_1 \subset \mathbb{V}_n$, $S_1 \in \{\mathbb{V}_n, \mathcal{C}_{R_0}\}$, find

$$T_S(A) := \arg\min_{T \in S} \|T - A\|, \quad \text{where} \quad S \in \{\mathcal{T}_r, \mathcal{C}_R, \mathcal{T}_{\mathcal{C}_R, r}\}. \quad (1)$$

Rem. $d = 2$: Celebrated theorem by E. Schmidt, 1907 on best bilinear approximation of $f(x, y)$ (mimics truncated SVD).
▷ **HOSVD, ALS** for best orthogonal **Tucker approximation**.
[De Lathauwer, De Moor, J. Vandewalle '00], (Leuven).

**Enhanced ALS** for canonical approximation - **Many contributions**.

▷ **General concept of tensor approximation in mathematical physics**.
[Beylkin, Mohlenkamp '02-'05], (Colorado, Ohio).

[Hackbusch, BNK, Tyrtyshnikov '03-'07], (Leipzig, Moscow).

▷ **Analytic methods** of tensor approximation in higher dimensions.
[Braess, Gavrilyuk, Hackbusch, BNK '05-'08], (Bohum, Eisenach, Leipzig).

▷ **Multigrid accelerated mixed** canonical-to-Tucker-to-canonical tensor approximation. **ALS via reduced HOSVD.** [BNK, Khoromskaia '08], (Leipzig).

▷ **Cross approximation** in \( \mathbb{R}^3 \). [Oseledets, Savostianov, Tyrtyshnikov '08], (Moscow).

▷ **Tensor representation of functions/operators** in the Hartree-Fock eq. and its iterative solution in tensor format.
[BNK, Khoromskaia, Flad '09], (Leipzig, Berlin).

▷ **Toward tensor methods for SPDEs** [BNK, Schwab '09] (Leipzig, Zurich).
Recent theory and numerics.

1. Tensor representation of $d$-variate functions/operators:
   - Multi-dimensional integral operators in $\mathbb{R}^d$,
   - Convolution, $\text{FFT}_d$ and Laplace transforms,
   - Elliptic Green’s functions, $(\Delta \pm \mu)^{-1}$.

2. Two-level Tucker-canonical multigrid accelerated tensor approximation: theory and algorithms.

3. Tensor truncated solvers for spectral/b.v. probl. in $\mathbb{R}^d$.

4. Electronic structure calculations: first results on solution of the 3D nonlinear Hartree-Fock eq. in tensor format.

5. Solving stochastic PDEs in tensor format (high-dimensional “stochastic” variable).

6. Preliminary numerical tests.
The Poisson-Boltzmann equation for electrostatic potential of protein

\[ \nabla \cdot \left[ \varepsilon(x) \nabla \phi(x) \right] - \varepsilon(x) h(x)^2 \sinh(\phi(x)) + 4\pi \rho(x)/kT = 0, \quad x \in \mathbb{R}^3. \]

If \( \varepsilon(x) = \varepsilon_0, \ h(x) = h, \ \rho(x) = \delta(x), \) then \( \phi(x) = \frac{e^{-h \|x\|}}{\|x\|}. \)


VILLIN (left); central slice and its rank-30 decomposition (middle-right).

Rank-30 Tucker approximation of FD solution on \( n \times n \times n \) grid (\( n \approx 150 \)), provides the relative accuracy \( 10^{-1} \div 10^{-2} \) in the Euclidean norm [E.A. Hayryan, V. Khoromskaia, 2009], in progress.
Aluminium cluster (14/172 atoms): 3D FEM* → Tucker ($r = 20$). B. Khoromskij, TRICAP 2009, 15.06.09


Linear transforms are reduced to 1D-operations + rank truncation.

Tensors $A_1$, $A_2$ in the canonical format

$$A_1 = \sum_{k=1}^{R_1} c_k u_k^{(1)} \otimes \ldots \otimes u_k^{(d)}, \quad A_2 = \sum_{m=1}^{R_2} b_m v_m^{(1)} \otimes \ldots \otimes v_m^{(d)}.$$  

1. Euclidean inner product (complexity $O(dR_1R_2n) \ll n^d$),

$$\langle A_1, A_2 \rangle := \sum_{k=1}^{R_1} \sum_{m=1}^{R_2} c_k b_m \prod_{\ell=1}^{d} \langle u_k^{(\ell)}, v_m^{(\ell)} \rangle.$$  

2. Hadamard product of $A_1$, $A_2$

$$A_1 \odot A_2 := \sum_{k=1}^{R_1} \sum_{m=1}^{R_2} c_k b_m \left( u_k^{(1)} \odot v_m^{(1)} \right) \otimes \ldots \otimes \left( u_k^{(d)} \odot v_m^{(d)} \right) \xrightarrow{TS}.$$  

3. Convolution of two 3rd order tensors $A_1$, $A_2$,

$$A_1 * A_2 = \sum_{k=1}^{R_1} \sum_{m=1}^{R_2} c_k b_m (u_m^{(1)} * v_k^{(1)}) \otimes (u_m^{(2)} * v_k^{(2)}) \otimes (u_m^{(3)} * v_k^{(3)}) \xrightarrow{TS}$$

with linear scaling in $n$, $O(R_1R_2n \log n) \ll n^3 \log n$ (3D FFT).
Truncated preconditioned iteration via tensor structured vectors and matrices in $S \in \mathbb{R}^{n^d} \rightleftharpoons \mathbb{R}^n \otimes ... \otimes \mathbb{R}^n$:

Solve BVPs in $S$: $A U = F$, 

\[ \tilde{U}_{m+1} = U_m - B^{-1}(A U_m - F), \quad U_{m+1} := T_S(\tilde{U}_{m+1}) \in S. \]

Solve EVPs in $S$: $A U = \lambda U$, 

\[ \tilde{U}_{m+1} = U_m - B^{-1}(A U_m - \lambda_m U_m), \]

\[ U_{m+1} := T_S(\tilde{U}_{m+1}) \in S, \]

\[ U_{m+1} := \frac{U_{m+1}}{||U_{m+1}||}, \quad \lambda_{m+1} = \langle A U_{m+1}, U_{m+1} \rangle_S. \]

$T_S$ - nonlinear projection onto tensor structured manifold $S$. 

$B^{-1}$ - tensor approximation of $(-\Delta + z)^{-1}$. 
Example 1. Negative Laplacian in $\Omega = (0, \pi)^d$.

$$(\lambda, u) \in \mathbb{R} \times H_0^1(\Omega) \setminus \{0\} : \quad -\Delta u = \lambda u.$$ 

$$\lambda_i = \sum_{\ell=1}^{d} i_{\ell}^2, \quad u_i = \prod_{\ell=1}^{d} \sin(i_{\ell} x_{\ell}), \quad i = (i_1, \ldots, i_d) \in \mathbb{N}^d.$$ 

The eigenvectors are exactly in the rank-1 tensor format.

Example 2. The Schrödinger equation for hydrogen atom,

$$(-\frac{1}{2}\Delta - \frac{1}{\|x\|})u = \lambda u, \quad x \in \Omega := \mathbb{R}^3.$$ 

The eigenpair with minimal eigenvalue is

$$u_1(x) = e^{-\|x\|}, \quad \lambda_1 = -0.5,$$

and $e^{-\|x\|}$ can be proven to have the low canonical rank.
Algorithm BTA \((\forall n \rightarrow T_{r,n})\): Cost \(O(n^{d+1})\).

Algorithm C_BTA \((C_{R,n}\rightarrow T_{C_{R,r}})\) has polynomial cost in \(R, n\),

\[
\text{For } n \geq R, \quad d = 3 : \quad O(R^2 n) + O(nr^4).
\]

Use the two-level Tucker-canonical format

\[
C_{R,n} \rightarrow T_{C_{R,r}} \rightarrow T_{C_{R',r}} \subset C_{R',n}, \quad R' < R.
\]

Level-I: compute the best rank-\(r\) orthogonal Tucker approximation with \(C_{R,n}\)-type input, so that the resultant core is represented in the \(C_{R,r}\) format.

Level-II: the small-size Tucker core in \(C_{R,r}\) is approximated by an element in \(C_{R',r}\) with \(R' < R\).
Thm. (Solving Problem 3.) [BNK, Khoromskaia '08]

(a) For \( A = \sum_{\nu=1}^{R} \xi_{\nu} u_{\nu}^{(1)} \otimes \ldots \otimes u_{\nu}^{(d)} \in \mathcal{C}_{R,n} \), the minimisation problem

\[ A \in \mathcal{C}_{R,n} \subset \mathbb{V}_{n} : \quad A_{(r)} = \text{argmin}_{T \in \mathcal{T}_{r,n}} \| A - T \|_{\mathbb{V}_{n}}, \]

is equivalent to the dual maximisation problem

\[ [Z^{(1)}, \ldots, Z^{(d)}] = \text{argmax}_{V^{(\ell)} \in \mathcal{M}_{\ell}} \left\| \sum_{\nu=1}^{R} \xi_{\nu} \left( V^{(1)} T u_{\nu}^{(1)} \right) \otimes \ldots \otimes \left( V^{(d)} T u_{\nu}^{(d)} \right) \right\|_{\mathbb{V}_{r}}^{2}. \]

(b) (reduced HOSVD of \( A \)). The maximizer is computed by the ALS iteration, with the initial guess via rank-\( r_{\ell} \) truncated SVD of the \( \ell \)-mode side-matrix \( U^{(\ell)} = [u^{(\ell)}_{1} \ldots u^{(\ell)}_{R}] \in \mathbb{R}^{n \times R} \) (\( \ell = 1, \ldots, d \)).

(c) (Error of RHOSVD). Let \( \sigma_{\ell,1} \geq \sigma_{\ell,2} \ldots \geq \sigma_{\ell,\min(n,R)} \) be the singular values of \( U^{(\ell)} \in \mathbb{R}^{n \times R} \) (\( \ell = 1, \ldots, d \)). Then the RHOSVD approx. of \( A \), \( A_{(r)}^{0} \), exhibits the error bound (cf. the complete \( O(n^{d+1}) \)-HOSVD, [De Lathauwer et al. 2000]),

\[ \| A - A_{(r)}^{0} \| \leq \| \xi \| \sum_{\ell=1}^{d} \left( \sum_{k=r_{\ell}+1}^{\min(n,R)} \sigma_{\ell,k}^{2} \right)^{1/2}, \quad \| \xi \| = \sqrt{\sum_{\nu=1}^{R} \xi_{\nu}^{2}}. \]
Multigrid accelerated method, [BNK, Khoromskaia ’08].

\( d = 3 \): Cost \( O(Rrn) \).

Main idea:

- Solve the sequence of approximation problems for \( A_n = A_{n_m} \) with \( n = n_m := n_02^m, m = 0, 1, ..., M \). Unigrid method via RHOSVD approximation of \( A_{n_0} \) only on the coarse grid.

- Use the coarse approximation of dominating subspaces.

- ALS iteration on the reduced data set over “most important fibers” (MIFs) of projected unfolding matrices, computed via maximal energy principle (on a coarse grid only).

- Multigrid → the localization of dominating subspaces via incomplete data.
[BNK '08], \( f_\kappa(x) = \frac{\exp(i\kappa \|x\|)}{\|x\|}, \ x \in \mathbb{R}^d, \ \kappa \in \mathbb{R}. \)

(a) Separable approximation of the “regularised” Helmholtz-type kernels

\[
f_{1,\kappa}(\|x\|) := \frac{\sin(\kappa \|x\|)}{\|x\|},
\]

\[
f_{2,\kappa}(\|x\|) := \frac{1}{\|x\|} - \frac{\cos(\kappa \|x\|)}{\|x\|} = \frac{2\sin^2\left(\frac{\kappa}{2} \|x\|\right)}{\|x\|}.
\]

**Complexity** of the rank-\(O(\kappa)\) canonical approximation, \(d = 3\),

\[O(|\log \varepsilon| (|\log \varepsilon| + \kappa)n) \ll O(\kappa^3 \log \kappa + n^3 \log n) \quad [\text{cf. Beylkin et al. '08}]\]

**High frequency regime:**

\( \kappa = Cn \Rightarrow O(n^2 \log n) \ll O(n^3 \log n). \)

(b) Separable approximation of the fundamental solution for \(\Delta\) in \(\mathbb{R}^d\),

\[f(x) := 1/\|x\|^{d-2}, \quad x \in \mathbb{R}^d.\]
**Theorem.** (Rank estimate for oscillating kernels.) [BNK ’08]

For given tolerance $\varepsilon > 0$, the function $f_{1,\kappa} : [0, \frac{2\pi}{\sqrt{d}}]^d \rightarrow \mathbb{R}$ allows the Tucker/canonical approximations, s.t.

$$\sigma(f_{1,\kappa}, S) \leq C\varepsilon \quad \text{with} \quad S = \{\mathbf{T}_r, \mathbf{C}_R\},$$

$$r \leq R \leq Cd(|\log \varepsilon| + \kappa), \quad r = (r, \ldots, r).$$

Let $f_1(t) = \frac{\sin^2(\kappa/2\sqrt{t})}{t}$, then the coefficients tensor for $f_{2,\kappa} : [0, \frac{2\pi}{\sqrt{d}}]^d \rightarrow \mathbb{R}$, w.r.t. the tensor product basis of p.w.c. basis-functions $\{\phi_i(x)\}$, and given by

$$G = [G_i]_{i \in \mathcal{I}} \quad \text{with} \quad G_i = \|x_i\|f_1(\|x_i\|) \int_{\mathbb{R}^d} \frac{1}{\|x\|} \phi_i(x) dx,$$

allows the Tucker/canonical approximations, providing the rank estimate

$$r \leq R \leq Cd^2|\log \varepsilon|(|\log \varepsilon| + \kappa).$$
Canonical approximation to $1/\|x\|^{d-2}$ for $d = 5$. Approx. error $\approx 10^{-6}$. 

Newton, dim=5, $1/|x|^3$, MaxCrank=25, grid=128
Canonical approximation of the Coulomb potential via \textit{sinc}-quadratures (solid lines).
Algebraically recompressed approximations (marked solid lines).
$L^2$-projection on p.w.c. basis functions over $n \times n \times n$ grid.

[Bertoglio, Hackbusch, BNK '08]
Example I: Helmholtz kernel in \( \mathbb{R}^3 \)  

Convergence history for the Tucker model applied to \( f_{2, \kappa}, \kappa \in [1, 15] \), with fixed accuracy \( \varepsilon > 0 \).
The Hartree-Fock equation

\[
\left[ -\frac{1}{2} \Delta - V(x) + \int_{\mathbb{R}^3} \frac{\rho(y)}{\|x - y\|} \, dy \right] \phi(x) - \frac{1}{2} \int_{\mathbb{R}^3} \frac{\tau(x, y)}{\|x - y\|} \phi(y) \, dy = \lambda \phi(x),
\]

\[\tau(x, y) = \sum_{i=1}^{N_e/2} \phi_i(x) \phi_i(y)\] - the electron density matrix,

\[\rho(y) = \tau(y, y)\] - the electron density,

\[\frac{1}{\|x\|}\] - the Newton potential,

\[V(x) = \sum_{\nu} \frac{Z_\nu}{\|x - x_{\nu}\|}\] - external nuclei potential.

**Challenging features:**

▷ Nonlinear equations

▷ Nonlocal (integral) operators.

▷ Large spatial grids in 3D.

▷ High accuracy.
Example II: Hartree potential on large grids

\[ V_H(x) := \int_{\mathbb{R}^3} \frac{\rho(y)}{|x - y|} \, dy = \left( \rho \ast \frac{1}{\| \cdot \|} \right)(x). \]

Represent orbitals in “approximating basis” \( \{ g_k \} \), e.g., the GTO basis,

\[
\rho(x) = \sum_{i=1}^{N/2} (\varphi_i)^2, \quad \varphi_i = \sum_{k=1}^{R_0} c_{i,k} g_k(x), \quad R_0 \approx 100,
\]

\[ g_k = (x - A_k)^{\beta_k} e^{-\lambda_k (x - A_k)^2}, \quad x \in \mathbb{R}^3. \]

\( O(n \log n) \)-computation of \( V_H \) and its Galerkin matrix in tensor format, on large \( n \times n \times n \) grids, error \( O(h^3) \), \( h = 1/n \).

Use Canonical-to-Tucker-to-canonical transform on a sequence of grids to reduces the initial rank, \( R_\rho \approx R_0^2 / 2 \).

[V. Khoromskaia, BNK '08].

Compared with MOLPRO analytic program.
Fast tensor convolution in $\mathbb{R}^3$ vs. FFT,

(Matlab, time/sec, linear scaling in $R_\rho$ and $n$), $R_\rho = 861$, $r = 15$.

<table>
<thead>
<tr>
<th>$n^3$</th>
<th>128$^3$</th>
<th>256$^3$</th>
<th>512$^3$</th>
<th>1024$^3$</th>
<th>2048$^3$</th>
<th>4096$^3$</th>
<th>8192$^3$</th>
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<td>55.4</td>
<td>582.8</td>
<td>$\sim 6000$</td>
<td>$-$</td>
<td>$-$</td>
<td>$-$</td>
<td>$\sim 2$ years</td>
</tr>
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<td>$C \ast C$</td>
<td>1.0</td>
<td>3.1</td>
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<td>43.7</td>
<td>127.1</td>
<td>368.6</td>
<td>700.2</td>
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</table>
Example II: Hartree potential on large grids

a) Absolute error of the tensor-product computation for the Hartree potential of the HO$_2$ molecule in the interval $\Omega = [-6, 6] \times \{0\} \times \{0\}$;

b) CPU times corresponding to $n \times n \times n$-grid, up to $n = 16000$. 
Coulomb (Galerkin) matrix is computed by tensor inner products in \( \{g_k\} \),

\[
J_{km} := \int_{\mathbb{R}^3} g_k(x)V_H(x)g_m(x)dx, \quad k, m = 1, \ldots R_0, \quad x \in \mathbb{R}^3.
\]

a) Electron density of \( \text{H}_2\text{O} \) in \( \Omega = [-4, 4] \times [-4, 4] \times \{0\} \).

c) Absolute approx. error for the Coulomb matrix \( \{J_{km}\} \) (\( \approx 10^{-6} \)).
[V. Khoromskaia '09], in preparation. Linear scaling in \( n \), cubic in \( R_0 \).

\[
K_{km} := -\frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} g_k(x) \frac{\tau(x, y)}{|x - y|} g_m(y) \, dx \, dy, \quad k, m = 1, \ldots R_0.
\]

Absolute \( L^\infty \)-error in the matrix elements of \( K \) for the density of \( \text{CH}_4 \) and pseudodensity of \( \text{CH}_3\text{OH} \).

Univariate grid size \( n = 1024, 4096 \). Approximation error \( O(h^3) \), \( h = 1/n \).
\[ g_\mu \in H^1(\mathbb{R}^3) : \quad \psi_i = \sum_{\mu=1}^{N_b} C_{\mu i} g_\mu, \quad i = 1, \ldots, N. \]

For \( C = \{ C_{\mu i} \} \in \mathbb{R}^{N_b \times N} \), and \( F(C) = H + J(C) - K(C) \), with Galerkin matrices in the approximating basis \( \{ g_\mu \} \),

\[ I \rightarrow S, \quad \mathcal{H} = -\frac{1}{2} \Delta + V_c \rightarrow H, \quad V_H \rightarrow J(C), \quad K \rightarrow K(C), \]

solve eigenvalue problem

\[ F(C)C = S \Lambda, \quad \Lambda = \text{diag}(\lambda_1, \ldots, \lambda_N) \]

\[ C^* SC = I_N. \]

Multilevel “fixed-point” tensor-truncated iteration:

initial guess \( C_0 \), for \( J = K = 0 \), grid size \( n = n_0, 2n_0, \ldots, 2^p n_0 \),

\[ \tilde{F}_k C_{k+1} = S C_{k+1} \Lambda_{k+1}, \quad \Lambda_{k+1} = \text{diag}(\lambda_1^{k+1}, \ldots, \lambda_N^{k+1}) \rightarrow \Lambda \]

\[ C_{k+1}^* S C_{k+1} = I_N, \]

where \( \tilde{F}_k, \ k = 0, 1, \ldots \), is specified by extrapolation over \( F(C_k), F(C_{k-1}), \ldots \) and \( J(C), K(C) \) are computed fast in tensor format.

[H.-J. Flad, V. Khoromskaia, BNK ’09], in preparation
▷ Multigrid convergence in eigenvalues (left).
▷ Convergence in effective iterations scaled to finest grid (right).
Linear scaling of the CPU time (per iteration) in the univariate grid size \( n \).
Example IV. Spectral problems in high dimensions

\[-\Delta u = \lambda u \quad \text{in} \quad [0, \pi]^d.\]

<table>
<thead>
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<th>$n + 1$</th>
<th>Time/it</th>
<th>$\delta \lambda$</th>
<th>$\delta u$</th>
<th>it.</th>
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<td>$2.0 \cdot 10^{-4}$</td>
<td>$1.5 \cdot 10^{-3}$</td>
<td>4</td>
</tr>
<tr>
<td>256</td>
<td>0.05</td>
<td>$1.6 \cdot 10^{-5}$</td>
<td>$9.4 \cdot 10^{-4}$</td>
<td>4</td>
</tr>
<tr>
<td>1024</td>
<td>0.12</td>
<td>$7.8 \cdot 10^{-7}$</td>
<td>$1.2 \cdot 10^{-4}$</td>
<td>5</td>
</tr>
<tr>
<td>4096</td>
<td>0.51</td>
<td>$4.9 \cdot 10^{-8}$</td>
<td>$3.4 \cdot 10^{-5}$</td>
<td>5</td>
</tr>
<tr>
<td>16384</td>
<td>2.2</td>
<td>$3.1 \cdot 10^{-9}$</td>
<td>$9.3 \cdot 10^{-6}$</td>
<td>5</td>
</tr>
<tr>
<td>65536</td>
<td>10.6</td>
<td>$1.9 \cdot 10^{-10}$</td>
<td>$2.8 \cdot 10^{-6}$</td>
<td>5</td>
</tr>
<tr>
<td>131072</td>
<td>22.3</td>
<td>$4.8 \cdot 10^{-11}$</td>
<td>$1.6 \cdot 10^{-6}$</td>
<td>5</td>
</tr>
</tbody>
</table>

Minimal $\lambda$ for 3D Laplacian on $n \times n \times n$ grids, $n = 2^p - 1$, $p = 6, 8, ..., 17$.

[Hackbusch, BNK, Sauter, Tyrtyshnikov '08]

<table>
<thead>
<tr>
<th>$d$</th>
<th>Time/it</th>
<th>$\delta \lambda$</th>
<th>$\delta u$</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>0.9</td>
<td>$3.1 \cdot 10^{-6}$</td>
<td>$4.5 \cdot 10^{-4}$</td>
</tr>
<tr>
<td>10</td>
<td>2.9</td>
<td>$3.1 \cdot 10^{-6}$</td>
<td>$3.8 \cdot 10^{-4}$</td>
</tr>
<tr>
<td>50</td>
<td>14.7</td>
<td>$3.1 \cdot 10^{-6}$</td>
<td>$3.1 \cdot 10^{-4}$</td>
</tr>
</tbody>
</table>

Minimal $\lambda$ for the $d$-Laplacian ($d = 3, 10, 50$), $n = 512$. [BNK '08-'09]
[BNK, Ch. Schwab '09]

Given an elliptic operator

$$\mathcal{A} := - \text{div} \left( a_M(y, x) \text{grad} \right)$$

and

$$f \in L^2(D), \quad D \in \mathbb{R}^d, \quad d = 1, 2, 3,$$

$$a_M(y, x)$$ is a smooth function of $$x \in D, \; y = (y_1, \ldots, y_M) \in \Gamma := [-1, 1]^M,$$

Find $$u_M \in L^2(\Gamma) \times H^1_0(D),$$ s.t.

$$\mathcal{A}u_M(y, x) = f(x) \quad \text{in} \; D, \quad \forall y \in \Gamma,$$

$$u_M(y, x) = 0 \quad \text{on} \; \partial D, \quad \forall y \in \Gamma.$$

For random field that is linear in the stochastic variable:

$$a_M(y, x) := a_0(x) + \sum_{m=1}^{M} a_m(x) y_m,$$

where $$a_m \in L^\infty(D), \; m = 0, \ldots, M,$$ are defined by the truncated Karhunen-Loéve expansion.
The tensor-truncated iterative method scales linearly in $M \leq 50$.

Variable coefficients with exponential decay ($\alpha = 1$, $n = 63$, $R \leq 5$),

$$a_m(x) = 0.5 e^{-\alpha m} \sin(mx), \quad m = 1, 2, \ldots, M, \quad x \in (0, \pi).$$

Rank approximation in tensor-truncated preconditioned iteration for solving sPDE with $d = 1$, $M = 10, 20$. 
Fundamental questions (no ultimate answers):

- **Is there a curse of dimensionality (amount of information)?**
  NO, for physically relevant data, cf. Kolmogorow’s paradigm.

- **Can we represent the basic operators in tensor format?**
  YES, for Green’s kernels, elliptic resolvent, convolution, \( f(A) \).

- **Can we solve the minimization problem (1) efficiently?**
  YES, the multigrid accelerated two-level approx., cross approx.

- **Can we expect the fast (exponential) convergence in the rank parameters \( R, r = \max r_\ell \)?**
  YES, for physically relevant data (solutions of basic equations).
  Sinc quadratures + algebraic “recompression“.

- **Can we solve the basic equations in \( \mathbb{R}^d \) on nonlinear manifold \( S \)?**
  YES, by tensor-structured methods.

  - SCF tensor-truncated iteration for the Hartree-Fock equation.
  - Linear EVPs in \( \mathbb{R}^d \).
  - Stochastic PDEs.