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*Everything should be made as simple as possible,
but not simpler.
A. Einstein (1879-1955)*

Prospects of Tensors Numerical Methods in Scientific Computing

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1. Motivating applications:

Bio/organic molecule systems: electronic structure, molecular dynamics.

FEM/BEM in \mathbb{R}^d : stochastic PDEs, atmospheric model., financial math.

Data mining: Machine learning, signal/image processing.

2. Computational bottleneck - "curse of dimension":

$O(N^d)$ -methods using $\underbrace{N \times N \times \dots \times N}_d$ grids (linear in volume size).

3. Methods based on separation of variables:

$O(dN)$ -tensor-structured methods to represent d -variate functions, operators, and for solving physical equations on rank-structured manifolds in \mathbb{R}^d , $d \geq 3$.

4. log-volume super-compressed approximation:

Quantics-TT approximation of N - d tensors, $N^d \rightarrow O(d \log N)$.

- Compute a pair $(\lambda, u) \in \mathbb{R} \times H_0^1(\Omega)$, s.t., $\langle u, u \rangle = 1$,

$$\begin{aligned}\mathcal{H}u &= \lambda u \quad \text{in } \Omega \in \mathbb{R}^d, \\ u &= 0 \quad \text{on } \partial\Omega.\end{aligned}$$

- Parabolic equations: Find $u : \mathbb{R}^d \times (0, \infty) \rightarrow \mathbb{R}$, s.t.

$$u(x, 0) \in H^2(\mathbb{R}^d) : \quad \sigma \frac{\partial u}{\partial t} + \mathcal{H}u = 0, \quad \mathcal{H} = \Delta_d + V(x_1, \dots, x_d).$$

- Elliptic (parameter-dependent) eq.: Find $u \in H_0^1(\Omega)$, s.t.,

$$\mathcal{H}u := -\operatorname{div}(A \operatorname{grad} u) + Vu = F \quad \text{in } \Omega \in \mathbb{R}^d.$$

Specific features:

- High spacial dimension: $\Omega = (-b, b)^d \in \mathbb{R}^d$ ($d = 2, 3, \dots, 100, \dots$).
- Multiparametric eq.: $A(\mathbf{y}, x)$, $u(\mathbf{y}, x)$, $\mathbf{y} \in \mathbb{R}^M$ ($M = 1, 2, \dots, 100, \dots, \infty$).
- Nonlinear, nonlocal (integral) operator $V = V(x, u)$, singular potentials.

1. Discretization in tensor product Hilbert space of N - d tensors, $\mathbb{V}_{\mathbf{n}} = \mathbb{R}^{\mathcal{I}}$, $\mathcal{I} = I_1 \times \cdots \times I_d$. Euclidean scalar product.
2. MLA in low separation rank tensor formats $\mathcal{S} \subset \mathbb{V}_{\mathbf{n}}$:

$$\mathcal{S} = \{\mathcal{C}_R, \mathcal{T}_{\mathbf{r}}, \mathcal{T}_{\mathcal{C}_R, \mathbf{r}}, TT[\mathbf{r}], QTT[\mathbf{r}], \mathcal{C}_{loc}, QTT_{loc}\}.$$

3. Efficient tensor truncation (projection),

$$T_{\mathcal{S}} : \mathcal{S}_0 \subset \mathbb{V}_{\mathbf{n}} \rightarrow \mathcal{S}, \quad \mathbf{n} = (N, \dots, N),$$

based on SVD + HOSVD + ALS/GRAD + multigrid.

4. Multilevel tensor-truncated preconditioned iteration.
5. Quasi-direct tensor-structured solvers.

Def. 1. Weakly (locally) coupled canonical N -($d + 1$) tensors, $\mathbf{V} \in \mathbb{R}^{J \times \mathcal{I}}$,

$$\mathbf{V} \in \mathcal{C}_{loc}[R] : \quad \mathbf{V}(j, \mathcal{I}) = \sum_{k=1}^R \bigotimes_{\ell=1}^d V_k^{(\ell)}(j), \quad V_k^{(\ell)}(j) \in \mathbb{R}^{I_\ell}, j \in J.$$

Def. 2. (Tensor Train/Chain format), $\text{TT}[\mathbf{r}]$ / $\text{TC}[\mathbf{r}]$.

Given the product index set $J := \times_{\ell=1}^d J_\ell$, $J_\ell = \{1, \dots, r_\ell\}$, and $J_0 = J_d$. The rank- \mathbf{r} tensor chain (TC) format

$$\text{TC}[\mathbf{r}, \mathbf{n}, d] \equiv \text{TC}[\mathbf{r}] \subset \mathbb{V}_{\mathbf{n}},$$

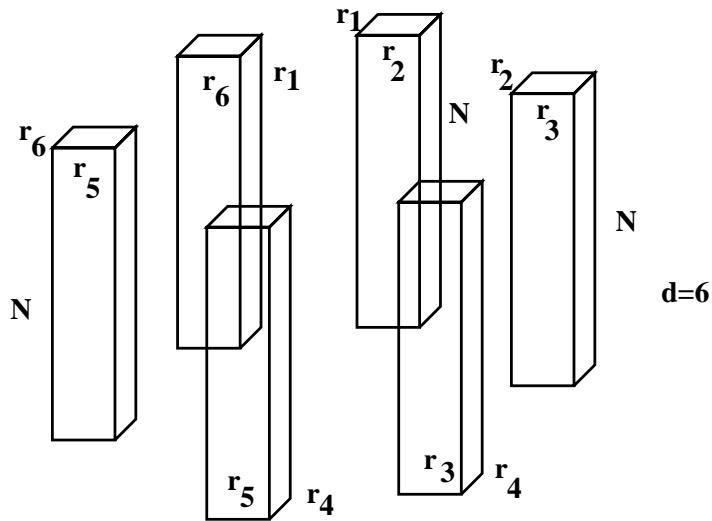
contains all $\mathbf{V} \in \mathbb{V}_{\mathbf{n}}$ that can be presented as the chain of contracted products of 3-tensors over (auxiliary) J ,

$$\mathbf{V} = \{\times_\ell\}_{\ell=1}^d \mathbf{G}^{(\ell)} \quad \text{with 3-tensors} \quad \mathbf{G}^{(\ell)} \in \mathbb{R}^{J_{\ell-1} \times I_\ell \times J_\ell}.$$

If $J_0 = J_d = \{1\}$ (disconnected chain), TC -format coincides with the Tensor-Train (TT) model, [Oseledets, Tyrtyshnikov '09].

TC - [BNK, Preprint 55/2009 MPI MiS, Leipzig]

$\underbrace{N \times N \times \dots \times N}_d$ -tensor in TC format: the d -fold contracted product of tri-tensors ($d = 6$).



Special case $r_6 = 1$: $\text{TT}[r] = \text{TC}[r]$ (disconnected chain).

Canonical embedding: $\text{TT}[r] \subset \text{TC}[r]$.

Lem. 1. (TC/TT: Storage, rank, concatenation, quasioptimality).

- (A) Storage: $\sum_{\ell=1}^d r_{\ell-1} r_\ell N \leq dr^2 N$ with $r = \max_\ell r_\ell$.
- (B) Rank bound, $r \leq \text{rank}(\mathbf{V})$, and canonical embeddings:
$$TT[\mathbf{r}] \subset TC[\mathbf{r}]; \quad \mathcal{C}_{R,\mathbf{n}} \subset TT[\mathbf{r}] \quad \text{with} \quad \mathbf{r} = (R, \dots, R).$$
- (C) Concatenation to higher dim.: $\mathbf{V}[d_1] \otimes \mathbf{V}[d_2] \rightarrow D = d_1 + d_2$.
- (D) SVD-based quasioptimal TT[r]-approx., $\mathbf{T} \in TT[\mathbf{r}]$,

$$\mathbf{V} \in \mathbb{V}_{\mathbf{n}} : \quad \|\mathbf{V} - \mathbf{T}\|_F \leq \left(\sum_{\ell=1}^d \varepsilon_\ell^2 \right)^{1/2}, \quad \varepsilon_\ell = \min_{\text{rank } B \leq r_\ell} \|V_{(\ell)} - B\|_F.$$

- (E) Direct SVD-based rank compression scheme.

Remarks toward the proof of Lem. 1, (D).

Quasioptimality via SVD-based approximation.

- ▷ Full-to-Tucker-HOSVD – [De Lathauwer et al. 2000].
- ▷ Canonical-to-Tucker-RHOSVD – [BNK, Khoromskaia '08].
- ▷ TT – [Oseledets, Tyrtyshnikov '09].
- ▷ Hierarchical dimension splitting – [Hackbusch, Kühn; Grasedyck '09].
- ▷ Quantics-TT – [BNK, 55/2009]; [Oseledets '09]; [BNK, Oseledets, 79/2009]
- ▷ QTT_{loc} – bounds on r_ℓ for some tensor classes,
applications to SPDEs (in the spirit of Def. 1).
- ▷ TC-approximation requires ALS iteration.

Quantics model: Vector/Tensor Tensorization to highest possible dim.

Lem. 2. [BNK '09] (Quantics folding of an exponential vector).

For a given $N = 2^L$, with $L \in \mathbb{N}_+$, and $c, z \in \mathbb{C}$, the exponential N -vector

$$\mathbf{X} := \{x_n := cz^{n-1}\}_{n=1}^N \in \mathbb{C}^N,$$

can be reshaped by the dyadic folding to the rank-1, $\underbrace{2 \times 2 \times \dots \times 2}_L$ -tensor,

$$\mathcal{F}_{2,1,L} : \mathbf{X} \mapsto \mathbf{A} = c \otimes_{p=1}^L \begin{bmatrix} 1 \\ z^{2^{p-1}} \end{bmatrix}, \quad \mathbf{A} : \{1, 2\}^{\otimes L} \rightarrow \mathbb{C}, \quad (2-L \text{ tensor}).$$

The trigonometric N -vector,

$$\mathbf{X} := \{x_n := c \sin(\alpha(n-1))\}_{n=1}^N,$$

can be reshaped to the $2-L$ tensor, of TT-rank 2, (Hint: $\sin z = \frac{e^{iz} - e^{-iz}}{2i}$).

Polynomial degree $p \rightarrow$ TT-rank p [Grasedyck '10].

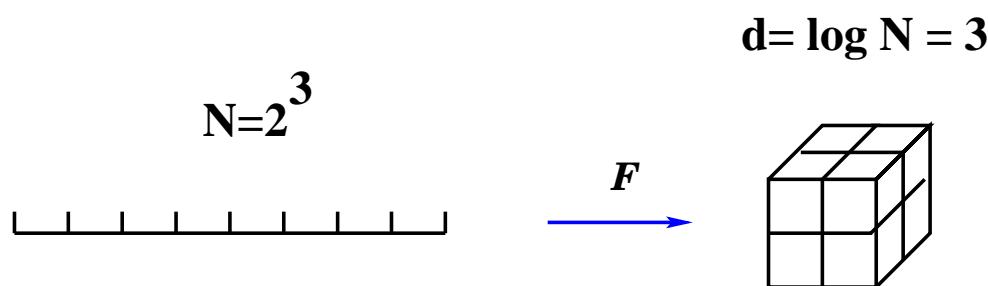
Benefit: Reduces the number of representation parameters $N \rightarrow 2 \log_2 N$.

Def. 3. Quantics + TT = QTT model (or QTC).

Ex. 1. For $d = 1$ and $p = 2, 3$, $\mathcal{F}_{q,1,p}$ folds an N -vector to a $N/q \times q$ -matrix or to $N/q^2 \times q \times q$, 3-tensor, respectively.

Ex. 2. Quantics folding of the exponential N -vector: $N = 8$, $L = 3$, $\mathbf{X} = [1 z z^2 z^3 z^4 z^5 z^6 z^7]^T \in \mathbb{C}^8$, $\mathcal{F}_{2,1,3}(\mathbf{X}) \in QC[1]$.

$$\mathcal{F}_{2,1,3} : \mathbf{X} \mapsto \mathbf{A} = \begin{bmatrix} 1 \\ z \end{bmatrix} \otimes \begin{bmatrix} 1 \\ z^2 \end{bmatrix} \otimes \begin{bmatrix} 1 \\ z^4 \end{bmatrix} \in \mathbb{C}^{2 \times 2 \times 2}.$$



[BNK '09] (Use TT-toolbox [Oseledets '09]).

The average splitting rank of the TC/TT model,

$$\bar{r} = \sqrt{\frac{1}{d} \sum_{\ell=1}^d r_{\ell-1} r_\ell}, \quad \text{Storage} \leq 2d\bar{r}^2 \log N.$$

Function-related N -vector: $F = \{f(a + (i - \frac{1}{2})h)\}_{i=1}^N, h = \frac{b-a}{N}$.

$N \setminus \bar{r}$	$e^{-\alpha x^2}, \alpha = 0.1 \div 10^2$	$\frac{\sin(\alpha x)}{x}, \alpha = 1 \div 10^2$	$1/x$	e^{-x}/x	$x, x^{10}, \sqrt[10]{x}$
2^{10}	3.2/2.8/2.8/2.2	4.0/4.7/5.5	4	3.5	1.9/2.7/3.9
2^{12}	3.1/2.9/2.9/2.6	3.8/4.8/5.6	4.2	3.8	1.9/2.6/3.9
2^{14}	2.9/2.8/2.8/2.8	3.6/4.7/5.5	4.2	3.8	1.9/2.5/3.9
2^{16}	2.8/2.7/2.8/2.8	3.6/4.5/5.4	4.2	5.3	1.9/2.4/3.9

Table 1: QTT₂-ranks of large f-r N -vectors.

$N \setminus \bar{r}$	$1/(x_1 + x_2)$	$e^{-\ x\ }$	$e^{-\ x\ ^2}$	$\Delta_2^{-1} \mathbf{1}, \varepsilon = 10^{-6}, 10^{-7}, 10^{-8}$
2^9	5.0	9.4	7.8	3.6/3.6/3.6
2^{10}	5.1	9.4	7.7	3.6/3.6/3.6
2^{11}	5.2	9.3	7.5	3.7/3.7/3.7

Table 2: QTT₂-ranks of functional $N \times N$ -matrices, $N = 2^p$.

N	128	256	512	1024
$1/\ x\ $	13.8	16.0	17.5	18.0
$\rho(x)$	32.0	40.0	45.8	48.6
$\rho * \frac{1}{\ \cdot\ }$	32.1	34.9	20.2	28.2

Table 3: QTT₂-ranks of $1/\|x\|$ -tensor, the Hartree potential $V_H = \rho * 1/\|\cdot\|$, and electron density ρ of CH₄ on $N \times N \times N$ grids.

Linear-log-log scaling by quantics tensor-tensorization to auxiliary (virtual) dimension $D = d \log N$.

Lem. 3. The N - d tensor \mathbf{A} of dimension $N^{\otimes d}$, $N = 2^L$,

$$A(i_1, \dots, i_d) = \frac{1}{i_1 + i_2 + \dots + i_d} \approx \sum_{k=-M}^M c_k e^{-t_k(i_1 + i_2 + \dots + i_d)},$$

can be approximated by a rank- $|\log \varepsilon|$ (i.e., $M = |\log \varepsilon|$), 2- D tensor of order $D = d \log N$, with storage demand

$$W = d|\log \varepsilon| \log N \ll N^d.$$

Proof. Lem. 1, Lem. 2 & sinc-quadrature approximation.

High dimension: $d = 2^{10}$, $N = 2^{20} \Rightarrow W = 20 \cdot 2^{10} |\log \varepsilon| \ll 2^{2 \cdot 10^4}$.

Basic MLA operation:

"Projection" onto the nonlinear manifold of rank-structured tensors, $\mathcal{S} \subset \mathbb{V}_n$.

Def. 3. (**Tensor truncation** $T_{\mathcal{S}} : \mathbb{V}_n \rightarrow \mathcal{S}$). Given $\mathbf{A} \in \mathbb{V}_n$,

$$T_{\mathcal{S}}(\mathbf{A}) := \underset{\mathbf{T} \in \mathcal{S}}{\operatorname{argmin}} \|\mathbf{T} - \mathbf{A}\|, \quad \mathcal{S} \in \{\mathcal{T}_r, \mathcal{C}_R, \textcolor{red}{TT[r]}, \textcolor{red}{QTT[r]}\}.$$

\mathcal{T}_r , \mathcal{C}_R , $QTT[r]$ are nonlinear sets \Rightarrow nonlinear approximation.

$T_{\mathcal{S}}$ for $\mathcal{S} \in \{TT, QTT\}$, and $\mathbf{A} \in \mathcal{S}_0 \supset \mathcal{S}$ allows the SVD-based quasioptimal approximation of $O(d)$ -complexity.

Operator $T_{\mathcal{S}}$ is an extension of the truncated SVD to $d > 2$.

Assumption: \mathcal{A} and \mathcal{B}^{-1} are of low matrix \mathcal{S} -rank.

► Solve elliptic BVP in \mathcal{S} : $\mathcal{A}\mathbf{U} = \mathbf{F}$,

$$\tilde{\mathbf{U}}_{m+1} = \mathbf{U}_m - \mathcal{B}^{-1}(\mathcal{A}\mathbf{U}_m - \mathbf{F}), \quad \mathbf{U}_{m+1} := \mathcal{T}_{\mathcal{S}}(\tilde{\mathbf{U}}_{m+1}) \in \mathcal{S}.$$

► Solve elliptic EVP in \mathcal{S} : $\mathcal{A}\mathbf{U} = \lambda\mathbf{U}; \langle \mathbf{U}, \mathbf{U} \rangle = 1$,

Green function iteration ($\mathcal{A} = \Delta_d + \mathcal{V}$),

$$\tilde{\mathbf{U}}_{m+1} = (\Delta_d - E_m Id)^{-1}\mathcal{V}\mathbf{U}_m, \quad \mathbf{U}_{m+1} := \mathcal{T}_{\mathcal{S}}(\tilde{\mathbf{U}}_{m+1})/\|\mathbf{U}_{m+1}\|,$$

and E_{m+1} is recomputed at each step as a Rayleigh quotient:

$$E_{m+1} = \langle \mathcal{A}\mathbf{U}_{m+1}, \mathbf{U}_{m+1} \rangle.$$

► Solve parabolic BVP in \mathcal{S} : $\frac{\partial \mathbf{U}}{\partial t} + \mathcal{A}\mathbf{U} = 0, \mathbf{U}_0 = \mathcal{T}_{\mathcal{S}}(\mathbf{U}(0))$.

The explicit solution operator by QTT-matrix exponential,

$$\mathbf{U}(t) = e^{-\mathcal{A}t}\mathbf{U}_0 \approx \mathcal{T}_{\mathcal{S}}(e^{-\mathcal{A}t})\mathbf{U}_0, \quad t \geq 0.$$

Electronic structure calculations.

Hartree-Fock equation

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

over $\phi_i \in H^1(\mathbb{R}^3)$, $\int_{\mathbb{R}^3} \phi_i \phi_j = \delta_{ij}$, $1 \leq i, j \leq N_{orb}$.

$\tau(x,y) = 2 \sum_{i=1}^{N_{orb}} \phi_i(x) \phi_i(y)$ - electron density matrix,

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

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

$V_c(x) = \sum \frac{Z_\nu}{\|x-x_\nu\|}$ - external potential, x_ν - centers of atoms.

- ▶ Multilevel tensor-structured iteration, mixed Tucker-canonical format, $N \times N \times N$ grids, $N \sim 10^4$.

[BNK, V. Khoromskaia, H.-J. Flad, Preprint 44/2009 MPI MiS], SISC, submitted,

[V. Khoromskaia, Preprint 25/2009 MPI MiS], CMAM 2010, to appear

[BNK, V. Khoromskaia, SISC, 31/4, 3002-3026, 2009].

Discretised GTO basis,

$$\bar{g}_\mu \in H^1(\mathbb{R}^3) : \quad \phi_i(x) = \sum_{\mu=1}^{R_0} c_{\mu i} \bar{g}_\mu(x), \quad i = 1, \dots, N \equiv N_{orb}.$$

► Compute Galerkin matrices in the approximating basis $\{\bar{g}_\mu\}$,

$$I_N \rightarrow S, \quad \mathcal{H} = -\frac{1}{2}\Delta + V_c \rightarrow H_0, \quad V_H \rightarrow J(C), \quad \mathcal{K} \rightarrow K(C),$$

and solve for $C = \{c_{\mu i}\} \in \mathbb{R}^{R_0 \times N_{orb}}$, and $F(C) = H_0 + J(C) - K(C)$,
the nonlinear eigenvalue problem

$$F(C)C = SC\Lambda, \quad \Lambda = \text{diag}(\lambda_1, \dots, \lambda_N)$$

$$C^*SC = I_N.$$

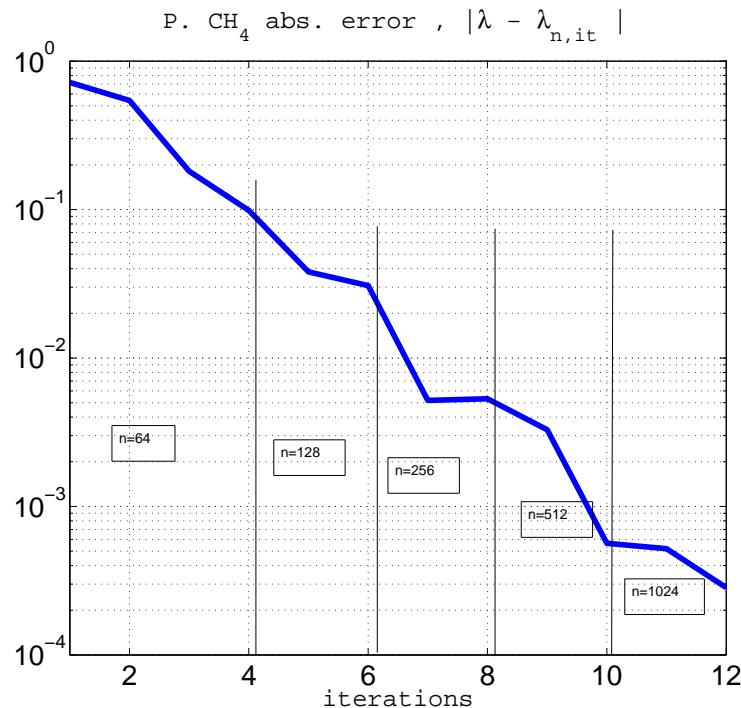
► Multilevel “fixed-point” tensor-truncated iteration, $k = 0, 1, \dots$:
initial guess C_0 , for $J = K = 0$, grid size $n = n_0, 2n_0, \dots, 2^p n_0$,

$$\tilde{F}_k C_{k+1} = SC_{k+1} \Lambda_{k+1}, \quad \Lambda_{k+1} = \text{diag}(\lambda_1^{k+1}, \dots, \lambda_N^{k+1}) \rightarrow \Lambda$$

$$C_{k+1}^* SC_{k+1} = I_N.$$

► DIIS iteration: Update \tilde{F}_k , by extrapolation over $F(C_k), F(C_{k-1}), \dots$,
where $J(C), K(C)$ are computed at $O(n \log n)$ -cost in tensor format.

- ▷ Discrete GTO Galerkin basis on $n \times n \times n$ grid.
- ▷ Multilevel tensor-truncated nonlinear SCF iteration for CH₄ (left).
 $r_T(\rho) = 22$, $r_T(\phi_i * \frac{1}{\|\cdot\|}) = 12$.
- ▷ Convergence in the effective iterations (right).



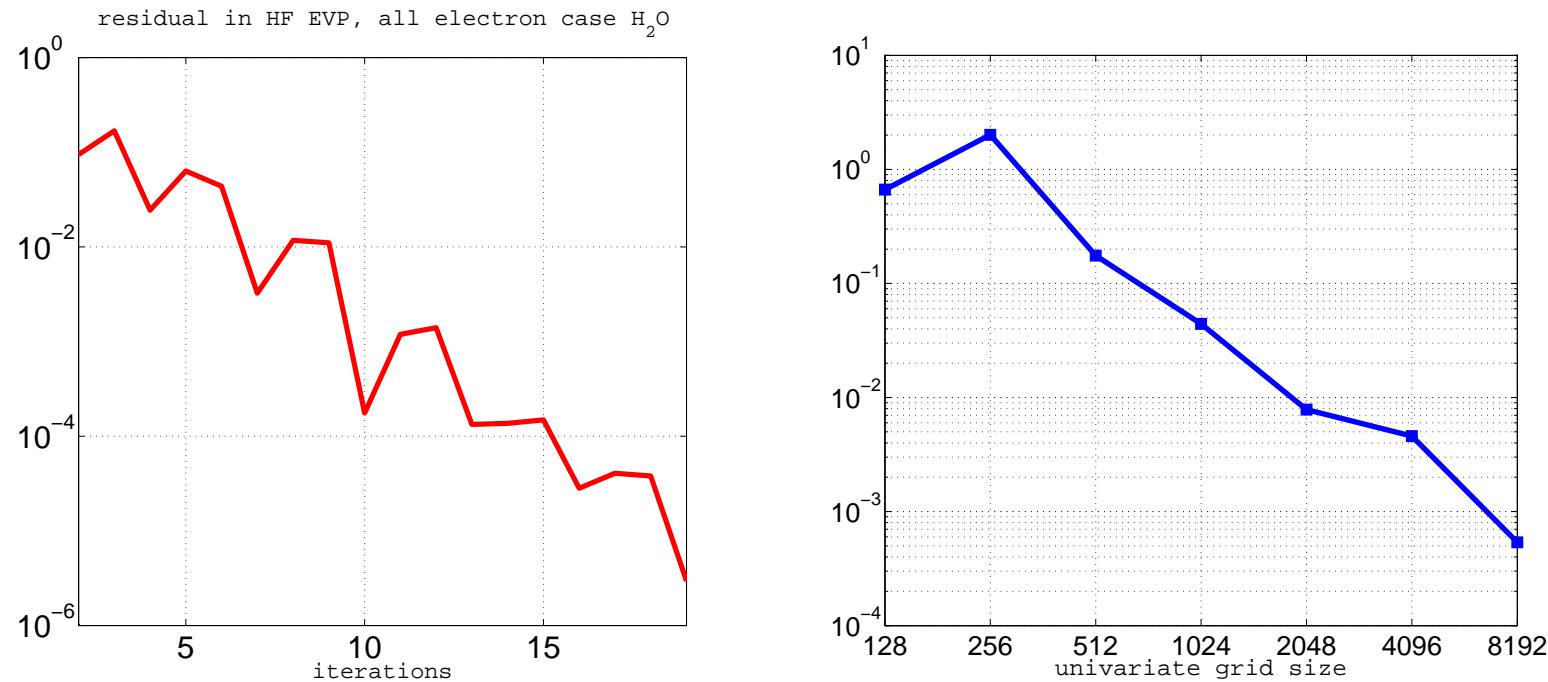


Figure 1: Multilevel SCF tensor iteration applied to the all electron case of H_2O (left), and energy convergence in n (right).

see for more details <http://personal-homepages.mis.mpg.de/vekh>

The Schrödinger equation for hydrogen atom,

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

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, $r = O(|\log \varepsilon|)$.

The Green function iteration and QTT₂ elliptic inverse by *sinc*-quadrature ($M = 20$). $N \times N \times N$ -grid, **Time = $O(\log N)$** .

[BNK, Oseledets, Preprint 79/2009 MPI MiS, Leipzig]

N	Time for 1 iter.	Iter.	Eigenvalue error
2^7	8.5	8	6.1e-03
2^8	13	8	1.5e-03
2^9	18	8	4.0e-04
2^{10}	25	8	1.0e-04

The Schrödinger equation for nuclei,

$$i\hbar \frac{\partial u}{\partial t} - \mathcal{H}u = 0, \quad \mathcal{H} = T + V,$$

with kinetic energy

$$T = - \sum_{\ell=1}^d \frac{\hbar^2}{2M_\ell} \Delta_{x_\ell}, \quad D(T) = H^2(\mathbb{R}^{3d}) \subset D(V), \quad x_\ell \in \mathbb{R}^3,$$

and a potential $V(x_1, \dots, x_d) \approx E(x_1, \dots, x_d)$ – potential energy surf. (PES)

PES, $E(x_1, \dots, x_d)$, is computed by **multiple solving of HF equation!**

► Spectral solvers

Multi-Configuration Time-Dependent Hartree method, [Meyer et al. 2000].

► Direct solver using Quantics-TT matrix exponential.

The solution operator $e^{-i\mathcal{H}t}$ could not be approximated by QTT-matrix exponential with uniform bound on the TT-ranks.

Introduce the regularization operator $\Sigma_p = \mathcal{H}^{-p} e^{-i\mathcal{H}t}$, $U_p = \mathcal{H}^p U(x, 0)$, $p \geq 1$, leading to stable QTT approximation,

$$U(x, t) = e^{-i\mathcal{H}t} U(x, 0) \approx (T_S \Sigma_p) T_S U_p, \quad t \geq 0.$$

Numerical example: quantum harmonic oscillator, $V(x) = \frac{1}{2}\|x\|^2$, $d = 1$, propagating the wave packet (exact eigenfunction) by $U(x, t) = U_n(x) e^{-i(n+1/2)t}$ on level $n = 0$, $t = 1.0$, $\varepsilon = 10^{-6}$, $p = 2$.

The average rank $rank_{QTT}$, indicates that QTT-ranks of both initial wave packet and the resultant solutions are about several ones.

N	$rank(\mathcal{H}^{-p} \cos(\mathcal{H}t))$	$rank(\mathcal{H}^{-p} \cos(\mathcal{H}t) U_p)$	$rank(U_p)$
2^8	33.8	3.7	4.7
2^9	33.2	3.7	4.7
2^{10}	32.5	3.6	4.9

Numerical cost is $= O(\log t \log N)$, N - spatial grid-size.

[BNK '10], Preprint 21/2010, MPI MiS.

$\Delta_d = \Delta_1 \otimes I_N \otimes \dots \otimes I_N + \dots + I_N \otimes I_N \dots \otimes \Delta_1 \in \mathbb{R}^{I^{\otimes d} \times I^{\otimes d}}$ - FD d -Laplacian,

$$\Delta_d U = F \quad \text{on} \quad N \times N \times \dots \times N - \text{grid.}$$

$$F = \bigotimes_{\ell=1}^d f_\ell, \quad f_\ell \in \mathbb{R}^N, \quad \text{rank}(F) = 1.$$

sinc-quadrature approx. + QTT₂-compression, $T_{\mathcal{S}} U := U_M$,

$$\Delta_d^{-1} F \simeq U_M := T_{\mathcal{S}} \sum_{k=-M}^M c_k \bigotimes_{\ell=1}^d \exp(-t_k \Delta_1) f_\ell, \quad \Delta_1 \in \mathbb{R}^{N \times N},$$

$$t_k = e^{k\mathfrak{h}}, \quad c_k = \mathfrak{h} t_k, \quad \mathfrak{h} = \pi/\sqrt{M},$$

with the exponential convergence rate

$$\|\Delta_d^{-1} F - U_M\|_\infty \leq C e^{-\pi\sqrt{M}}, \quad (\text{or } \leq C e^{-\pi M / \log M}).$$

Complexity in canonical format: $O(d|\log \varepsilon|^2 N) \ll N^d$.

$\text{rank}(\Delta_d) = d$.

$\text{rank}_{TT}(\Delta_d) = 2$, for any $d \geq 2$.

Matrix representation in QTT₂-format.

$N \setminus \bar{r}$	$e^{-\alpha\Delta_1}, \alpha = 0.1, 1, 10, 10^2$	Δ_1^{-1}	$\text{diag}(1/x^2)$	$\text{diag}(e^{-x^2})$
2^9	6.2/6.8/9.7/11.2	6.2	5.1	4.0
2^{10}	6.3/6.8/9.5/10.8	6.3	5.3	4.0
2^{11}	6.4/6.8/9.0/10.4	6.2	5.5	4.1

Table 4: QTT₂-matrix-ranks of $N \times N$ -matrices, $N = 2^p$.

[BNK Preprint 55/2009, MPI MiS, Leipzig]

Numerical complexity in QTT-format: $W = O(d|\log \varepsilon|^2 \log N)$.

N	Precomp	Time for sol	Residue	Relative L_2 error
2^5	1.70	1.57	9.1e-06	8.9e-06
2^6	2.56	1.98	7.8e-06	7.3e-06
2^7	4.19	2.45	7.3e-06	7.1e-06
2^8	6.14	2.98	6.6e-06	7.0e-06
2^9	8.37	3.52	8.7e-06	7.0e-06
2^{10}	10.81	4.02	9.4e-06	7.0e-06

Table 5: Solving 100D Poisson equation in C-QTT₂.

Find $u_M \in L^2(\Gamma) \times H_0^1(D)$, s.t.

$$\begin{aligned} \mathcal{A}u_M(\mathbf{y}, x) &= f(x) \quad \text{in } D, \quad \forall \mathbf{y} \in \Gamma, \\ u_M(\mathbf{y}, x) &= 0 \quad \text{on } \partial D, \quad \forall \mathbf{y} \in \Gamma, \end{aligned}$$

$$\mathcal{A} := -\operatorname{div}(a_M(\mathbf{y}, x) \operatorname{grad}) \quad \text{and} \quad f \in L^2(D), \quad D \in \mathbb{R}^d, \quad d = 1, 2, 3,$$

$a_M(\mathbf{y}, x)$ is smooth in $x \in D$, $\mathbf{y} = (y_1, \dots, y_M) \in \Gamma := [-1, 1]^M$, $M \leq \infty$.

Additive case

$$a_M(\mathbf{y}, x) := a_0(x) + \sum_{m=1}^M a_m(x)y_m, \quad a_m \in L^\infty(D), \quad M \rightarrow \infty,$$

via the truncated Karhunen-Loéve expansion.

Log-additive case

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

Canonical: [BNK, Ch. Schwab, Preprint 9/2010 MPI MiS Leipzig]

H-Tucker: [D. Kressner, C. Tobler, ETH Zuerich, 2010]

QTT: ?

A parametric linear system

$$A(y)u(y) = f, \quad f \in \mathbb{R}^N, \quad u(y) \in \mathbb{R}^N. \quad (1)$$

Additive case

$$A(y) = A_0 + \sum_{m=1}^M A_m y_m,$$

where A_m are $N \times N$ matrices, N - grid size in x .

A 1D grid $\{y_m^{(k)}\}$, $k = 1, \dots, n$, $1 \leq m \leq M$, n - grid size in $y = (y_1, \dots, y_M)$.

Assembled linear system

$$\mathbb{A}\mathbf{u} = \mathbf{f},$$

where \mathbb{A} is a $Nn^M \times Nn^M$ matrix, \mathbf{v} and \mathbf{g} are vectors of length Nn^M .

For the additive case,

$$\mathbb{A} = A_0 \times I \times \dots \times I + A_1 \times D_1 \times I \times \dots \times I + \dots + A_M \times I \times \dots \times D_M,$$

where D_m , $m = 1, \dots, M$, is $n \times n$ diagonal matrix with positions of collocation points $\{y_m^{(k)}\}$, $k = 1, \dots, n$ on the diagonal,

$$\mathbf{f} = f \times e \times \dots \times e, \quad e = (1, \dots, 1)^T \in \mathbb{R}^n.$$

Piece of theory:

Let $v = (-\Delta_x^{-1})f$, and $\sigma_m = \|a_m\| / (\sum_{m=1}^M \|a_m\|) > 0$,

define $b_m(y_m, x) = \sigma_m a_0(x) + a_m(x)y_m$.

Prop. 1. ([BNK, 21/2010 MPI MiS]) With $d = 1$, assume that

$\text{grad}_x u_M(y, x) \in C(D)$ for all $y \in \Gamma$, $\text{grad}_x v(x) \in C(D)$, $b_m(y_m, x) \geq 0$, and there exists $a_{min} > 0$, such that,

$$(A) \quad a_{min} \leq a_0(x) < \infty,$$

$$(B) \quad \left| \sum_{m=1}^M a_m(x)y_m \right| \leq \gamma a_{min} \text{ with } \gamma < 1, \text{ and for } |y_m| < 1 \text{ (} m = 1, \dots, M \text{)}.$$

⇒ The additive case: $O(M|\log \varepsilon|Nn)$ -complexity; The log-additive case: $O(MNn)$ -complexity.

Proof. Use the idea in [Dolgov, BNK, Tyrtyshnikov, '10] with $d = 1$. Then there exist positive constants $c_k, t_k \in \mathbb{R}$, s.t. (sinc-quadrature)

$$\left\| \text{grad}_x u_M(y, x) - C_0 - \sum_{k=-K}^K c_k \prod_{m=1}^M e^{-t_k b_m(y_m, x)} \text{grad}_x v(x) \right\|_{L^\infty} \leq C e^{-\beta K / \log K},$$

where $\beta > 0$ and C do not depend on M and K .

Quadrature discretization of parametric PDE in the log-additive case.

Prop. 2. ([BNK, Oseledets, '10] in preparation)

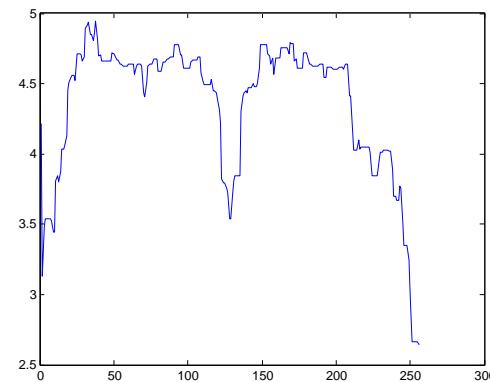
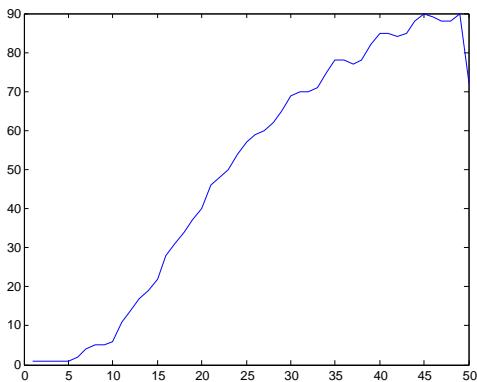
Each tensor-element $A(i, j, y)$ of size n^M , $i, j = 1, \dots, N$, has canonical decomposition of rank $\lesssim 3^d$. There exists canonical approximation to the assembled $Nn^M \times Nn^M$ matrix \mathbb{A} with $\text{rank}(\mathbb{A}) \lesssim 3^d N$, independently of n and M .

Numerics in additive case, $d = 1$, $\varepsilon = 10^{-6}$:

(Left) Global QTT-ranks, $O(M)$, for the solution vs. mode number

(Right) Local QTT-ranks, $O(1)$, for the solution tensor at grid points,

$M = 50$, $n = 256$, quadratic decay of coefficients $a_m(x) = 1/m^2 \sin(mx)$.



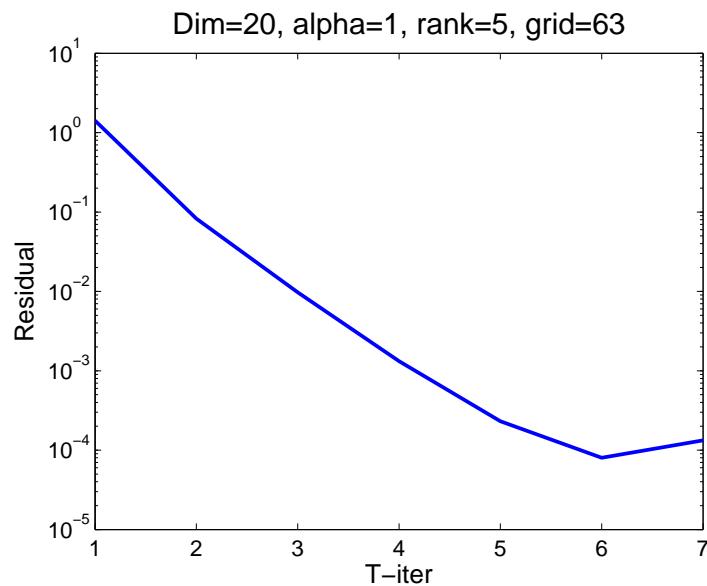
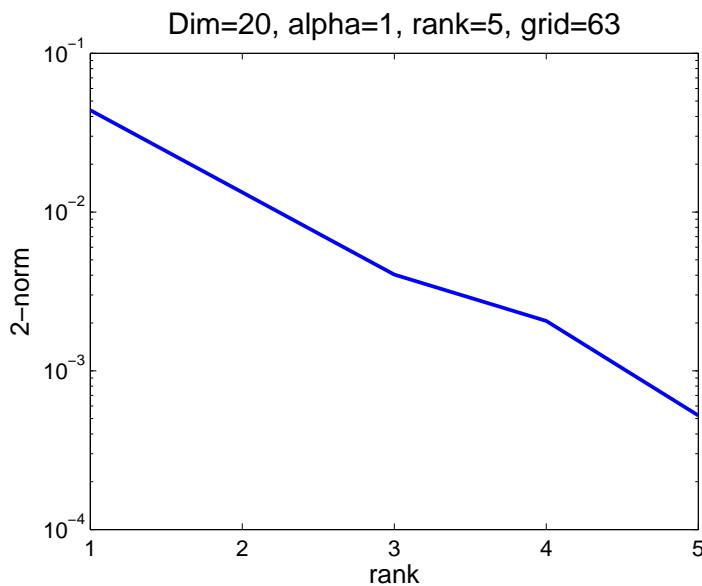
[BNK, Ch. Schwab, Preprint 9/2010 MPI Leipzig]

► Preconditioned tensor-truncated iteration in $(d + M)$ -dimensional parametric space. Canonical format, $M \leq 100$.

\mathcal{S} -truncated preconditioned iteration for solving sPDE $\mathcal{A}(y)U(y) = F$, $N^{\otimes(M+d)}$ -grid, $d = 1$, $M = 20$ ($\mathcal{S} = \mathcal{C}_R$, $\mathcal{B} := \mathcal{A}(0)^{-1}$).

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

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



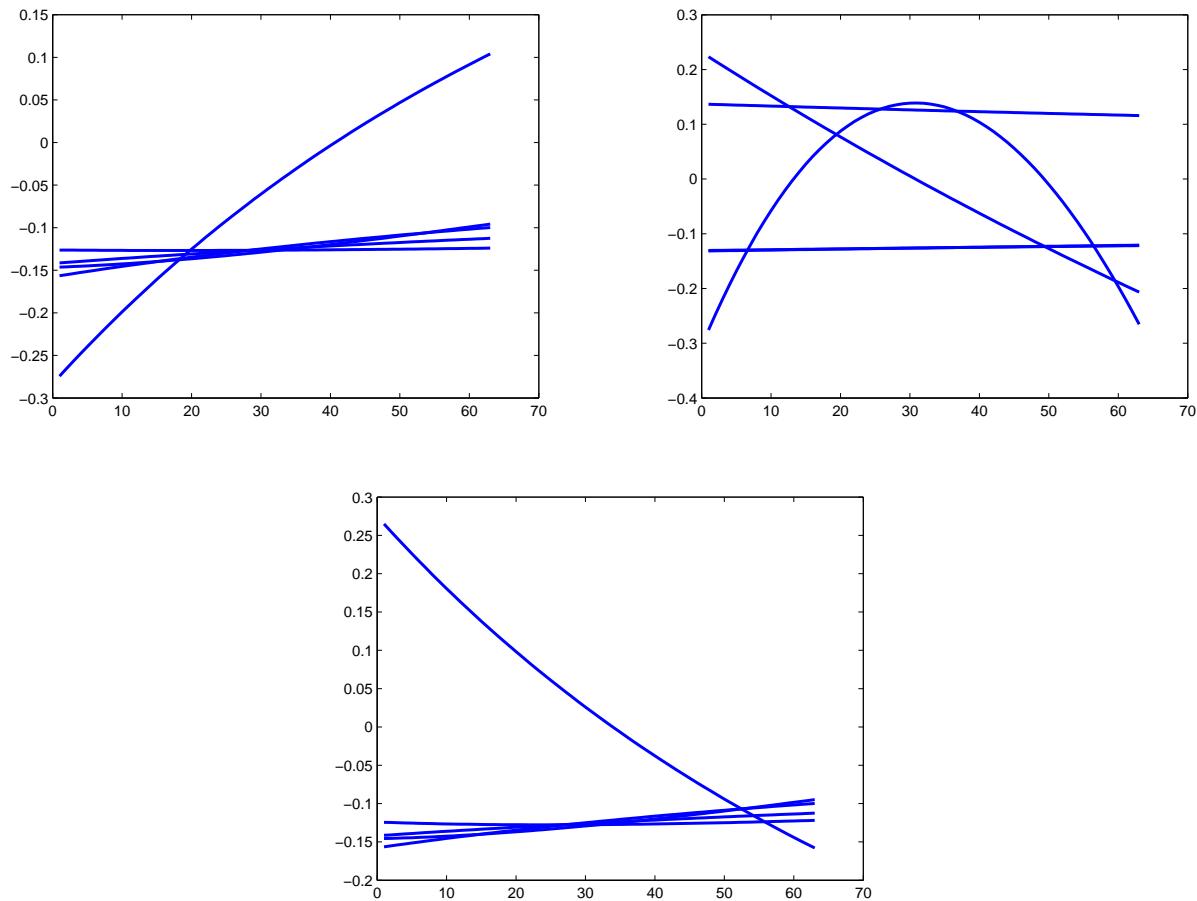


Figure 2: Examples of ℓ -mode canonical vectors ($\ell = 1, 2, 3$) for solutions of sPDE with $M = 20$, $R = 5$, and $a_m(x) = 0.5 e^{-\alpha m} \sin(mx)$.

“... the tensor-structured numerical methods have proved their value in application to various function related tensors arising in quantum chemistry and in the traditional FEM/BEM modeling—the tool apparently works and gives the promise for future use in challenging high-dimensional applications.”

Thank you very much!