Tensor numerical approach to space-time approximation of multi-dimensional parabolic equations

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Tensor methods vs. the “curse of dimensionality”: $N^d \rightarrow dN \rightarrow d \log N$?

PDE based applications in higher dimensions:

- Elliptic (parameter-dependent) BV/spectral problems:
  \[ u \in H^1_0(\Omega) : \quad \mathcal{H}u := -\text{div}(a \text{grad } u + uv) + Vu = F \quad (= \lambda u) \quad \text{in } \Omega \in \mathbb{R}^d. \]

- Parabolic-type dynamics: Find $u : \mathbb{R}^d \times (0, T) \rightarrow \mathbb{R}$, s.t.
  \[ u(x, 0) \in H^2(\mathbb{R}^d) : \quad \sigma \frac{\partial u}{\partial t} + \mathcal{H}u = F, \quad \sigma \in \{1, i\}. \]

Computational challenges:

Multi-dimensionality, multi-parametric problems, huge grids in $\mathbb{R}^d$ and in $t \in [0, T]$, multi-dimensional integral transforms (convolution), high oscillations in coefficients, redundancy in data representation.

Big Data $\not\equiv$ Big Knowledge! (curse of redundancy) $\Rightarrow$ Knowledge $= o(\text{Data})$?

Parallelization issues
1929, P.A.M. 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.*

1961, R. Bellman: *In view of all that we have said in the foregoing sections, the many obstacles we appear to have surmounted, what casts the pall over our victory celebration? It is the curse of dimensionality, a malediction that has plagued the scientist from earliest days.*

► **Low-rank nonlinear tensor approximation vs. information redundancy.**

1927-1966, Hitchcock, Tucker: *Canonical (CP) and Tucker tensor formats* in chemometrics.


2003, Dirac-Frenkel molecular dynamics on rank-1 tensor manifold.

Since 2006: *Tensor numerical methods* for PDEs in $\mathbb{R}^d$.

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Outline of the talk

1. Big-data compression via separation of variables: basic tensor formats
2. Range-separated tensor format: reduced model for many-particle interactions
3. Quantized-TT tensor approximation (QTT) of logarithmic complexity
4. $O(\log n)$ numerical quadratures by simple QTT algebraic operations
5. Elliptic PDEs with highly oscillating coefficients in log-complexity: tensor approximation vs. asymptotic homogenization
6. PDEs on complex geometry: Low-rank approximation in iso-geometric analysis
7. $d$-dimensional dynamics: time stepping vs. equations in $2 + 1, 3 + 1, \ldots, d + 1$
   - QTT integration for retarded potential IE (wave equation)
   - Rank estimates
   - Heat eqn., Fokker-Planck, chemical master equations
Separable representation in tensor-product Hilbert space

Euclidean vector space \( V_n = \mathbb{R}^{n_1 \times \ldots \times n_d} = \bigotimes_{\ell=1}^d \mathbb{R}^{n_\ell}, \) \( n = (n_1, \ldots, n_d), \)

\[ V = [v_i] \in V_n : \langle W, V \rangle = \sum_i w_i v_i, \quad i = (i_1, \ldots, i_d) : i_\ell \in \{1, \ldots, n_\ell\}. \]

Separable representations in \( V_n \) via rank-1 tensors:

\[ V = [v_{i_1 \ldots i_d}] = v^{(1)} \otimes \ldots \otimes v^{(d)} \in V_n : v_{i_1 \ldots i_d} = \prod_{\ell=1}^d v^{(\ell)}_{i_\ell}. \]

Storage: \( \text{Stor}(V) = \sum_{\ell=1}^d n_\ell \ll \dim V_n = \prod_{\ell=1}^d n_\ell \quad (nd \ll n^d). \)

The scalar product reduces to univariate operations

\[ \langle W, V \rangle = \langle v^{(1)} \otimes \ldots \otimes v^{(d)}, v^{(1)} \otimes \ldots \otimes v^{(d)} \rangle = \prod_{\ell=1}^d \langle w^{(\ell)}, v^{(\ell)} \rangle v^{(\ell)}. \]

Fast multilinear algebra: \( d \)-dimensional Hadamard product, contraction, convolution product, addition etc. all reduce to 1D-operations!

Low-parametric separable representations: canonical, Tucker, MPS (TT) formats

Most commonly used tensor formats extend rank-\( R \) matrices:

\( d = 2 : \quad V = \sum_{k=1}^R u_k v_k^T \equiv G_1 G_2^T \equiv UDV^T \in \mathbb{R}^{m \times n}. \)

- Canonical (CP) tensors (multidimensional rank-\( R \) representation) [Hitchcock ’27].
- The orthogonal Tucker decomposition (multidimensional truncated SVD) [Tucker ’66]
- Matrix product states (MPS) factorization [S. White ’92 et al.] ⇒ Variants of MPS: Tensor train (TT) [Oseledets, Tyrtyshnikov ’09]; Hierarchical Tucker (HT) [Hackbusch, Kühn ’09].

Def. Canonical \( R \)-term representation in \( V_n \): \( V \in \mathcal{C}_R(V_n), \)

\[ V = \sum_{k=1}^R v_k^{(1)} \otimes \ldots \otimes v_k^{(d)}, \quad v_k^{(\ell)} \in \mathbb{R}^{n_\ell}. \]

Advantages: Storage = \( dRN \), simple multilinear algebra, but hard for approximation.
Orthogonal Tucker decomposition

**Def.** Rank $r = (r_1, \ldots, r_d)$ Tucker tensors: $V \in \bigotimes_{\ell=1}^d T_\ell \subset \mathbb{V}_n$, $V^{(\ell)} \in \mathbb{R}^{n_{\ell} \times r_\ell}$

$$V = \sum_{k_1, \ldots, k_d=1}^r b_{k_1 \ldots k_d} V_k^{(1)} \otimes \cdots \otimes V_k^{(d)} = B \times_1 V^{(1)} \times_2 \cdots \times_d V^{(d)}; \quad T_\ell = \text{span}\{V_k^{(\ell)}\}_{k=1}^r \subset \mathbb{R}^{n_\ell}

**Storage:** $drN + r^d$, $r = \max r_\ell \ll N = \max n_\ell$. For functional tensors $r = O(\log N)$.

Basics of tensor numerical approximation [BNK, CMAM ’06], [BNK, Khoromskaia ’07]:
Low-rank decomposition of functional tensors, e.g. for $v(x) = e^{-||x||} \frac{1}{||x||} e^{-||x||}$:

$$\|V - V_r\| \leq e^{-cr}.$$

Matrix Product States (Tensor Train) factorization

**Def.** MPS (TT) format: Given $r = (r_1, \ldots, r_d)$, $r_d = 1$. $V = [v_i] \in TT[r] \subset \mathbb{V}_n$ is parametrized by contracted product of tri-tensors in $\mathbb{R}^{r_{\ell-1} \times n_\ell \times r_\ell}$,

$$v_{i_1 \ldots i_d} = \sum_\alpha G^{(1)}_{\alpha_1} [i_1] G^{(2)}_{\alpha_1 \alpha_2} [i_2] \cdots G^{(d)}_{\alpha_{d-1}} [i_d] \equiv G^{(1)}[i_1] G^{(2)}[i_2] \cdots G^{(d)}[i_d],$$

$G^{(\ell)}[i_\ell]$ is an $r_{\ell-1} \times r_\ell$ matrix, $1 \leq i_\ell \leq n_\ell$. **Storage:** $dr^2 N \ll N^d$.

$$d = 5: A = [a_{i_1i_2i_3i_4i_5}] \in \mathbb{R}^{n_{i_1} \times n_{i_2} \times n_{i_3} \times n_{i_4} \times n_{i_5}}. \text{ For } r = 1 \text{ all formats coincide!}

1D (univariate) function related vectors $f = \{f(x_i)\} \in \mathbb{R}^N$ are non-compressible ?

**Find a hidden low-rank tensor structure in large functional vectors and matrices !**
Range-separated (RS) tensor format for approximating funct. with multiple cusps

**Figure:** Villin protein (left). Short- and long-range parts of the reference Newton kernel $1/\|x\|$. 

[Benner, Khoromskaia, BNK '16]

- Long range interaction potential in the large $N_0$-particle system, $x_k \in \mathbb{R}^3$, $k = 1, \ldots, N_0$, and the radial function $p(\|x\|)$ (say, $p(\|x\|) = 1/\|x\|$)

$$P(x) = \sum_{\nu=1}^{N_0} z_k p(\|x - x_k\|), \quad z_k \in \mathbb{R}, \quad x_k, x \in \Omega = [-b, b]^3,$$

- The interaction energy of the system of $N_0$ charged particles

$$E_N = E_N(x_1, \ldots, x_N) = \frac{1}{2} \sum_{j=1}^{N} z_j \sum_{k=1, k \neq j}^{N} \frac{z_k}{\|x_j - x_k\|}.$$  \(1\)

RS canonical/Tucker/TT formats: beneficial properties


**Definition**

(RS-canonical (Tucker, TT) tensors). The RS-canonical tensor format defines the class of $d$-tensors $A \in \mathbb{R}^{n_1 \times \cdots \times n_d}$, represented as a sum of a rank-$R$ CP tensor $U$ and a cumulated CP tensor generated by localized $U_0$, s.t. $\text{rank}(U_{\nu}) = \text{rank}(U_0) \leq R_0$, $U_\nu = \text{Replica}(U_0)$,

$$A = \sum_{k=1}^{R} \xi_k u_k^{(1)} \otimes \cdots \otimes u_k^{(d)} + \sum_{\nu=1}^{N_0} c_{\nu} U_{\nu}, \quad \text{with} \quad \text{diam}(\text{supp}U_{\nu}) \leq n_0 = O(1).$$

**Theorem**

The storage size for RS-canonical tensor is estimated by

$$\text{Stor}(A) \leq dRn + (d + 1)N_0 + dR_0 n_0.$$

Each entry of an RS-CP tensor can be calculated at $O(dR + dR_0 n_0)$ cost.

For $\varepsilon$-rank of the Tucker approximation to the long-range CP tensor $U$, $r_0 = \text{rank}_{Tuck}(U)$:

$$|r_0| \leq C b \log^{3/2}(\|\log(\varepsilon/N_0)\|), \quad \text{rank}_{\text{Can}}(U) \leq |r_0|^2.$$
The "curse of dimensionality" ⇒ "blessing dimensions"!

\[ F_{N=2^3} \rightarrow L=\log N=3 \]

**[BNK '09] Quantized Tensor Approximation** (QTT) of functional \( N \)-vectors \( (N = 2^L) \).

\[ \text{Isometry } Q_L : [x_i]_{i=1}^N =: x \rightarrow A := [a_j] \in Q_L := \bigotimes_{\ell=1}^L \mathbb{R}^2, \]

\[ a_j := x_i, \quad i \mapsto j \in \{1,2\}^\otimes L : \quad i - 1 = \sum_{\ell=1}^L (j_\ell - 1)2^{\ell-1} \quad \text{(binary coding)}. \]

TT approximation of quantized image in \( Q_L \) ⇒ QTT method

Storage in QTT tensor format scales logarithmically in \( N = 2^L \),

\[ 2r^2 L \ll 2^L. \]

**QTT-approxim. theory: Why the super-compressed QTT-approximation does a job?**

**Thm. [BNK '09-'10].** QTT-approximation of functional \( N \)-vectors in \( O(\log N) \)-op. \( N = 2^L \).

- For quantized exponential \( N \)-vector: \( \text{rank}_{QTT}(x) = \text{rank}_{\text{Can}}(Q_L(x)) = 1 \),

\[ x := \{z^{n-1}\}_{n=1}^N \in \mathbb{C}^N \mapsto \bigotimes_{\ell=1}^L \left[ \frac{1}{z^{2^\ell-1}} \right] \in \bigotimes_{\ell=1}^L \mathbb{C}^2, \quad z \in \mathbb{C}. \]

- For quantized sin and cos \( N \)-vector: \( \text{rank}_{\text{Can},C}(x) = \text{rank}_{\text{QTT},\mathbb{R}}(x) = 2 \),

\[ x := \{
\sin(\omega h(n-1))\}_{n=1}^N \in \mathbb{C}^N, \quad h = 1/(N-1), \quad \forall \omega \in \mathbb{C}. \]

- QTT of a polynomial of degree \( m \), \( \text{rank}_{QTT}(P_m) \leq m + 1. \) ⇒ P.w. polynomials.

- Smoothly modulated multiply replicated functions.

- Gaussian \( e^{-\lambda x^2} \) has small \( \varepsilon \)-rank in QTT and QCan formats: \( r = O(\| \log \varepsilon \|) \).

- Approx. \( I(\omega, f) = \int_{\Omega} f(x)e^{i\omega g(x)} \, dx \) as a function of frequency \( \omega \) [BNK, Sauter, Veit 12-'15]

- Contribution to QTT approx. of functions [BNK, Oseledets, Dolgov, Grasedyck, Kazeev, Schwab]

- Numerical observation: \( 2^L \times 2^L \) 1D-Laplacian reshapes to a low TT-rank [Oseledets '09]
Example: $d$-dimensional discrete Laplacian as the Kronecker product sum

$$\Delta_d = \Delta_1 \otimes I \otimes \ldots \otimes I + I \otimes \Delta_1 \otimes I \otimes \ldots \otimes I + \ldots + I \otimes I \otimes \ldots \otimes \Delta_1 \in \mathbb{R}^{N^d \times N^d},$$

$\Delta_1 = \text{tridiag}\{-1, 2, -1\} \in \mathbb{R}^{N \times N}$, $I$ is the $N \times N$ identity.

- Canonical/Tucker representation: $\text{rank}_{CP}(\Delta_d) = d$, $\text{rank}_{Tuck}(\Delta_d) = 2$.
- TT/QTT representation: $\text{rank}_{TT}(\Delta_d) = 2$, $\text{rank}_{QTT}(\Delta_d) \leq 4$, $\forall d$.

$$\Delta_d = [\Delta_1 \ I] \propto \begin{bmatrix} I & 0 \\ \Delta_1 & I \end{bmatrix} \propto \begin{bmatrix} I \\ \Delta_1 \end{bmatrix}.$$

- [Kazeev, BNK ’10] Explicit QTT representation: $\text{rank}_{QTT}(\Delta_1) = 3$, $\text{rank}_{QTT}(\Delta_1^{-1}) \leq 5$.

$$\Delta_1 = \begin{bmatrix} I & J' \\ J & \end{bmatrix} \propto \begin{bmatrix} I & J' \\ J & \end{bmatrix} \propto \begin{bmatrix} 2l - J - J' \\ -J \\ -J' \end{bmatrix}.$$

$l = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \quad J = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}.$

“$\propto$” is a regular matrix product of block core matrices, blocks being multiplied by means of tensor product.

Beyond Galerkin: Nonlinear approximation in low-rank tensor formats

Approximation problem: Given $A \in \mathbb{V}_n$ (in general, $A \in \mathbb{S}_0 \subset \mathbb{V}_n$), find

$$T_r(A) := \arg\min_{X \in S} \|X - A\|,$$ where $S \subset \{T_r, C_R, \text{MPS/TT}[r]\}$.

Quasi-optimal (nonlinear) tensor approx. is based on: SVD, QR, Cholesky + ALS iter.

- SVD-based HOSVD for Tucker tensors [De Lathauwer et al. 2000]
- SVD-based HOSVD for MPS/TT tensors [Vidal ’06]

Tucker and MPS/TT ranks:

$$T_r := \{A \in \mathbb{V}_n : \text{rank}\ A^{(p)} \leq r_p\} : \ A^{(p)} = [a(j_1 j_2 \ldots j_{p-1} ; j_p ; j_{p+1} \ldots j_d)].$$

$$\text{TT}[r] := \{A \in \mathbb{V}_n : \text{rank}\ A^{[p]} \leq r_p\} : \ A^{[p]} = [a(j_1 j_2 \ldots j_d ; j_{p+1} \ldots j_d)].$$

Canonical rank can not be presented as a matrix rank $\Rightarrow$ unstable approximation :(

- Rank reduction in the canonical format. Reduced HOSVD:

Canonical $\leftrightarrow$ Tucker $\leftrightarrow$ canonical ALS for the Tucker core [BNK, Khoromskaia, SISC ’08].
I. QTT based quadratures of $O(\log n) = O(|\log \varepsilon|)$ complexity

- Quantized integrand $f(x)$ and weight function $w(x)$ with moderate QTT-ranks.
  The rectangular $n$-point quadrature, $n = 2^L$, $|I - I_n| = O(n^{-\alpha})$, Cost = $O(r^2 \log n)$.
  $$\int_{-1}^{1} w(x)f(x)dx \approx I_n(f) := h \sum_{i=1}^{n} w(x_i)f(x_i) = \langle W, F \rangle_{QTT}, \quad W, F \in \otimes_{i=1}^{L} \mathbb{R}^2.$$  

- Retarded potentials: [BNK, Sauter, Veit, CMAM 2011].
- Twofold-QTT: fast quadratures for highly oscillating integrals + QTT in $\omega$.

II. Asymptotic homogenization for elliptic PDEs with oscillating coefficients

[BNK, Repin: RJNAMM ’15]

Traditional FEM-Galerkin p.w.l. approximation in $\Omega = (0,1)^d$:

Find $u_\epsilon \in H^1_0(\Omega)$: $-\text{div}(a_\epsilon \nabla u_\epsilon) = f \quad \text{in } \Omega, \quad f \in L^2(\Omega), \quad (2)$

with oscillating or lattice-structured/replicated coefficients in $\Omega = \cup_i \Pi_i^\epsilon$,

$$a_\epsilon(x) := \tilde{A}\left(\frac{x - x_i}{\epsilon}\right) \quad \text{for } x \in \Pi_i^\epsilon - \text{scaled unit cell}.$$  

- Homogenization methods suggest asymptotically $\|u_\epsilon - u_{homo}\| \leq C\sqrt{\epsilon}$ as $\epsilon \to 0$.

Challenges: "Defected" periodic coeff.; Moderate $\epsilon$; Huge grids: $n^d \approx (n_0/\epsilon)^{-d}$.

Assumptions:

(A) $a_\epsilon(x)$ and "homogenized coeff." $a_0(x) = \frac{1}{2}(a^+(x) + a^-(x))$, have low QTT rank. $a^+(x)$ and $a^-(x)$ are the upper and lower majorants of $a_\epsilon(x)$.

(B) Solution of the “homogenized” equation $A_0u_0 = f$ is cheap. $a_0(x) \mapsto A_0.$
computational scheme: Solve the FEM-Galerkin approximation of (2)
\[ A_\varepsilon u_\varepsilon = f, \quad A_\varepsilon \in \mathbb{R}^{N^d \times N^d}, \quad u_\varepsilon, f \in \mathbb{R}^{N^d}, \quad N = 2^L \] (3)
in quantized tensor space $\mathbb{Q}_L$ by the rank-truncated preconditioned iteration:
\[ u_0 = A_0^{-1} f : \quad (E + \beta A_0^{-1} A_\varepsilon - E) u \equiv (E + B) u = \beta u_0, \quad \beta > 0, \]
assuming that $\|B\| = q < 1$ for $B = \beta A_0^{-1} A_\varepsilon - E$, and rank$_{QTT}(B)$ is small.

Given tol. $\delta > 0$, $u_0 \in \mathbb{Q}_L^{(r)}$:
\[ u_{k+1} = T_{QTT, \delta} (\beta u_0 - B u_k) \mapsto u_\delta, \quad k = 0, 1, 2, \ldots \]
\[ \|u_{k+1} - u_k\| \leq q^k \|u_0\| \] up to the truncation level $\delta > 0$.

QTT rank-truncated iteration of log-cost $O(\log N)$ vs. homogenization method

<table>
<thead>
<tr>
<th>Grid size $2^L$</th>
<th>$2^{13}, (it)$</th>
<th>$2^{14}, (it)$</th>
<th>$2^{15}, (it)$</th>
<th>$2^{16}, (it)$</th>
<th>$2^{17}, (it)$</th>
<th>$r(a_\varepsilon)$</th>
<th>$r(u_\delta)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C + \sin(\omega x)$</td>
<td>0.97, (5)</td>
<td>1.2, (5)</td>
<td>1.3, (5)</td>
<td>2.0, (6)</td>
<td>2.1, (6)</td>
<td>2.67</td>
<td>3.7</td>
</tr>
<tr>
<td>4-steps coef.</td>
<td>3.4, (9)</td>
<td>4.3, (9)</td>
<td>4.5, (9)</td>
<td>6.7, (9)</td>
<td>14.3, (14)</td>
<td>2.9</td>
<td>4.96</td>
</tr>
<tr>
<td>$C + \sin(\omega x^2)$</td>
<td>5.3, (5)</td>
<td>10.0, (6)</td>
<td>9.95, (6)</td>
<td>11.98, (6)</td>
<td>16.2, (5)</td>
<td>7.53</td>
<td>8.24</td>
</tr>
</tbody>
</table>

CPU sec., iter. history, QTT-ranks, $\omega = 1/\varepsilon = 2\pi 64$, $\delta_{QTT} = 10^{-7}$: $\|u_{\varepsilon} - u_\delta\|_0 \leq 10^{-7}$, $\|u_{\varepsilon} - u_\delta\|_1 \leq 10^{-6}$.

Precond. Steepest Descent in QTT-truncated iterations for the periodic, step-, and cubically-oscillating coef.
2D diffusion coefficients \(a(\epsilon(x))\), rhs, and the respective solutions: 400x400-grid in 5 sec.

\(f_1(x, y) = \sin(2x)\sin(2y);\) \(f_2(x, y) = \sin(2x)\).

III. Tensor approach to Iso-Geometric Analysis (IGA): toward dynamics


Figure: The yeti footprint domain, parameterized by 21 quadratic B-spline patches. Patch segmentation (left), control grids (middle) and the (absolute) Jacobian determinant are shown. On the left picture \(\text{rank}(\det \nabla G)\) and \(\max(\text{rank}(q_{k,\ell}), k, \ell \in \{1, 2\})\) are given. \(\epsilon = 10^{-10}\).
IGA: Matrix generation via patch-wise low-rank representation

FEM-Galerkin p.w.l. approximation in $\Omega \in \mathbb{R}^d$:

$$\text{Find } u \in H^1_0(\Omega) : \quad -\text{div}(a(x)\nabla u) = f \quad \text{in } \Omega, \quad f \in L^2(\Omega).$$

Figure: The Jacobian determinant values of the selected patch (Fig. 2) on the domain (left). The graph and control net in parameter domain (right).

IV. Temporal problems: Time stepping vs. global $x - t$ schemes in $d + 1$

Problem 1. Complex-time molecular Schrödinger eq. in QMD, $d = 3N$.

$$i \frac{\partial \psi}{\partial t} = H\psi = (-\frac{1}{2} \Delta_d + V)\psi, \quad \psi(x, 0) = \psi_0(x), \quad x \in \mathbb{R}^d,$$

$V : \mathbb{R}^d \rightarrow \mathbb{R}$ is (given) approximation to the potential energy surface (PES).

Problem 2. Real-time evolution. The Fokker-Planck equation

$$\psi(0) = \psi_0, \quad \frac{d\psi}{dt} = -A\psi; \quad A\psi = -\varepsilon \Delta \psi + \text{div}(\psi v), \quad \psi : \mathbb{R}^d \rightarrow \mathbb{R},$$

$v : \mathbb{R}^d \rightarrow \mathbb{R}^d$ is a given velocity field. $\psi(t) \rightarrow \psi_* : A\psi_* = 0$ (small eigs. of $A$)

Example 1’. Heat equation in $\mathbb{R}^d \times [0, T]$:

$$\frac{d\psi}{dt} = -\Delta \psi + f, \quad \psi(0) = \psi_0.$$ 

Problem 3. Chemical master equation for joint probability density $P(x, t)$,

$$P(x, 0) = P_0, \quad \frac{dP(x, t)}{dt} = A P(x, t), \quad x \in \mathbb{R}^{n_1 \times \ldots \times n_d}.$$

Problem 4. Wave equation in unbounded exterior domain (Dirichlet problem)

$$\partial^2_{tt} \psi - \Delta \psi = 0 \quad \text{in } \Omega \times [0, T], \quad \psi(\cdot, 0) = \partial_t \psi(\cdot, 0) = 0 \quad \text{in } \Omega \in \mathbb{R}^3.$$
Main approaches (all methods approximate $e^{-tH}\psi_0$!)

**Time integrators**
- Sparse grids in $(x, t)$: [Schwab et al.; Griebel et al.]
- Dirac-Frenkel projection onto Tucker/TT/QTT-manifold $S$,
  $$\langle \frac{dy}{dt} - Hy, \delta y \rangle = 0, \quad \delta y \in T_y S.$$  
  [Meyer et al. ’03; Lubich et al. ’07–’15]
- Wave equation in exterior domain: Tensor quadrature for retarded potentials
  [BNK, Sauter, Veit ’11]
- Time stepping by implicit scheme in TT/QTT + ALS/DMRG local solver,
  [Dolgov, BNK, Oseledets ’11; Schwab et al. ’12]

**Global time-space schemes in $d + 1$**
- Time-space separation by QTT-Cayley transform, rank bounds [Gavrilyuk, BNK ’11]
- QTT-Tucker + ALS-type solver on global $(x, t)$ tensor manifold
  [Dolgov, BNK ’12–14]

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**Wave equation: Retarded potential integral equation via QTT integration**

[BNK, Sauter, Veit: CMAM ’11] + work in progress ...

$\Omega \subset \mathbb{R}^3$ – a Lipschitz domain, $\Gamma = \partial \Omega$. Homogeneous wave equation

$$\partial_t^2 u - \Delta u = 0 \quad \text{in } \Omega \times [0, T]; \quad u = g \quad \text{on } \Gamma \times [0, T].$$

In applications, $\Omega$ is often the unbounded exterior of a bounded domain.

We employ an ansatz as a *single layer potential* for the solution $u$

$$u(x, t) := S\varphi(x, t) := \int_\Gamma \frac{\varphi(y, t - \|x - y\|)}{4\pi\|x - y\|} d\Gamma_y, \quad (x, t) \in \Omega \times [0, T].$$

$S$ is referred to as *retarded single layer potential* (the retarded time argument $t - \|x - y\|$ which connects time and space variables).

The boundary integral equation for unknown density $\varphi$,

$$\int_\Gamma \frac{\varphi(y, t - \|x - y\|)}{4\pi\|x - y\|} d\Gamma_y = g(x, t) \quad \forall (x, t) \in \Gamma \times [0, T]. \quad (4)$$
QTT-Cayley transform method

Dynamics and spectrum of high-dim. Hamiltonians [Gavrilyuk, BNK ’11]

\[ \psi(t) = \sum_{p=0}^{\infty} L_p^0(t) u_p \equiv i(H + il)^{-1} \sum_{p=0}^{\infty} L_p^0(t) G^p \psi_0, \quad t \in [0, T], \]

\[ G = H(H + il)^{-1}, \quad L_p - \text{Laguerre polynomials. Recursion for } u_p, \]

\[ u_0 = i(H + il)^{-1} \psi_0, \quad u_{p+1} = G u_p, \quad p = 0, 1, \ldots \]

The \( m \)-term truncated series representation

\[ \psi_m(t) = \sum_{p=0}^{m} L_p^0(t) u_p. \quad (5) \]

Def. \( f = \sum a_k \varphi_k(x) \) is called \( H \)-analytic if there is \( C = C(f) > 0 \), s.t.

\[ \| H^n f \| = \left( \sum_{k=0}^{\infty} a_k^2 \lambda_k^{2n} \right)^{1/2} \leq C^n n! \quad \text{for } n = 1, 2, 3, \ldots \]

where \( \{ \varphi_k, \lambda_k \} \) is the eigenpair of \( H = H^* \).

Rank bounds

Rem. For \( H \)-analytic vector \( f \) the power series \( \sum_{n=0}^{\infty} \frac{s^n}{n!} \| H^n f \| =: \| f \|_{s,H} \) possesses a positive convergence radius \( r > 0 \), i.e., \( \| f \|_{s,H} < \infty \) if \( 0 \leq s < r \).

Lem. Let \( \psi_0 \) be \( H \)-analytical, then for every fixed \( s > 0 \), and fixed \( T > 0 \), s.t. \( \| \psi_0 \|_{s,H} < \infty \), the \( \psi_m(t) \) converges exponentially in \( m \),

\[ \| \psi(t) - \psi_m(t) \| \leq c m^{-1/12} e^{-c_1 \frac{3m}{m}} \| \psi_0 \|_{s,H}, \quad t \in [0, T] \]

where \( c, c_1 > 0 \) are independent of \( m \).

Lem. QTT-rank of a tensor \( U = [\psi_m(t_1), \ldots, \psi_m(t_{N_t})]_{k=1}^{N_t}, \quad t_k = k \Delta t \), is bounded by

\[ \text{rank}_{QTT}(U) \leq \sum_{p=0}^{m} (p + 1) \text{rank}_{QTT} G^p(\psi_0). \]

For the harmonic oscillator:

\[ \text{rank}_{QTT}(U) \leq C m^2 \text{rank}_{QTT}(\psi_0). \]
The energy spectrum is recovered by FFT of autocorrelation function
\[ a(t) = \langle \psi_m(t), \psi(0) \rangle, \quad S(E) = \int_0^\infty a(t)e^{iEt} dt. \]

Simultaneous time-space QTT decomposition of complexity
\[ O(\log N_t \log N m^4 (\text{rank}_{QTT}(G^m\psi_0))^2), \quad m = O(\log^p \varepsilon). \]

Difficulties on examples of the molecular Schrödinger, Fokker-Planck and master equations:
- Even the low-rank Hamiltonian does not guarantee the low rank of the evolving solution!
- The Hamiltonian operator might not be well-separable (convection-diffusion).
- Boundary conditions (layer) may enforce rank instabilities (approximate b.c.).
- Large mode size (quantization).

High-dim. spectral calculations for the Henon-Heiles Hamiltonians (QMD)

[BNK, Oseledets ’11] Perturbed harmonic oscillator
\[ H = -\frac{1}{2} \Delta + \frac{1}{2} \sum_{k=1}^d q_k^2 + \lambda \sum_{k=1}^{d-1} \left( q_k^2 q_{k+1} - \frac{1}{3} q_k^3 \right), \quad \text{rank}_{TT}(H) \leq 3, \quad \text{rank}_{QTT}(H) \leq 4. \]

The energy spectrum is recovered by FFT of autocorrelation function
\[ a(t) = \langle \psi_m(t), \psi(0) \rangle, \quad S(E) = \int_0^\infty a(t)e^{iEt} dt. \]
Discretization on global QTT-tensor manifold in space-time

Given \( A, f_k \) in the TT/QTT format, apply Crank-Nicolson,

\[
(I + \frac{\tau}{2} A)y_{k+1} = (I - \frac{\tau}{2} A)y_k + \frac{\tau}{2}(f_k + f_{k+1}) =: F_{k+1}.
\]

(A) Time stepping by DMRG-TT iter. for solving

\[
(I + \frac{\tau}{2} A)y_{k+1} = F_{k+1}.
\]

(B) Global \( O(\log N_x \log N_t) \) block-AMEn solver in QTT-Tucker format:

\[
y_{k+1} - y_k + \frac{\tau}{2} A y_{k+1} + \frac{\tau}{2} A y_k = \frac{\tau}{2}(f_k + f_{k+1}).
\]

Solve the huge global \( N_x^d \times N_t \) system in QTT format by AMEn iteration

\[
\begin{bmatrix}
I + \frac{\tau}{2} A \\
-I + \frac{\tau}{2} A & I + \frac{\tau}{2} A & & & \\
& -I + \frac{\tau}{2} A & I + \frac{\tau}{2} A & & \\
& & & \ddots & \ddots & \ddots \\
& & & & -I + \frac{\tau}{2} A & I + \frac{\tau}{2} A
\end{bmatrix}
\begin{bmatrix}
y_1 \\
y_2 \\
\vdots \\
y_N
\end{bmatrix}
= \begin{bmatrix}
(I - \frac{\tau}{2} A) y_0 \\
0 \\
\vdots \\
0
\end{bmatrix}
+ \frac{\tau}{2}
\begin{bmatrix}
f_0 + f_1 \\
f_1 + f_2 \\
\vdots \\
f_{N-1} + f_N
\end{bmatrix}.
\]

Heat equation: global \((d+1)\)-scheme vs. time stepping

As a “sanity” test we consider the heat equation

\[
\frac{\partial u}{\partial t} - \Delta u = f \quad \text{in} \quad \Omega = [0, 1]^2,
\]

\[u(0) = g : \quad u|_{\partial \Omega} = 0.
\]

(A) The case of a smooth analytic solution (refinement of the grids).

Choose \( f = 0 \), \( g(x_1, x_2) = \sin(\pi x_1)\sin(\pi x_2) \).

The analytical solution at the time \( t \): \( u^*(x_1, x_2) = g(x_1, x_2) \exp(-2\pi^2 t) \).

The time interval is \([0, 1/2]\), the residual tolerance for the TT-solve algorithm: \(10^{-6}\).

Table: \( \frac{||u - u^*||_F}{||u||_F} \) versus the spatial \( N_x \) and time \( N_t \) grid sizes at \( t = 1/2 \).

<table>
<thead>
<tr>
<th>( N_t ) ( \times ) ( N_x )</th>
<th>( 2^8 )</th>
<th>( 2^9 )</th>
<th>( 2^{10} )</th>
<th>( 2^{11} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( 2^7 )</td>
<td>4.7598e-03</td>
<td>4.8515e-03</td>
<td>4.8746e-03</td>
<td>4.8803e-03</td>
</tr>
<tr>
<td>( 2^8 )</td>
<td>1.8271e-04</td>
<td>2.7475e-04</td>
<td>2.9786e-04</td>
<td>3.0363e-04</td>
</tr>
<tr>
<td>( 2^{11} )</td>
<td>1.0380e-04</td>
<td>1.1745e-05</td>
<td>1.1363e-05</td>
<td>1.7152e-05</td>
</tr>
<tr>
<td>( 2^{13} )</td>
<td>1.2171e-04</td>
<td>2.9652e-05</td>
<td>6.5401e-06</td>
<td>7.8656e-07</td>
</tr>
</tbody>
</table>

The convergence is faster than the theoretical bound \( O(N_t^{-2} + N_x^{-2}) \) of the Crank-Nicolson - FD scheme. The solution time of the block scheme is almost independent on \( N_t, N_x \) (100 – 200 milliseconds for any test in Table) since the QTT ranks are uniformly bounded by a small constant.
Heat equation: non-regular rhs

(B). \( f(x_1, x_2) = g = 1, x_1, x_2 \in (0, 1) \), i.e. discontinuous at the boundary. The time step should be small to resolve transitional processes near \( \Gamma \), otherwise, as the second-order scheme is not monotonous, the oscillations occur, leading to large tensor ranks.

\[ \begin{align*}
t \in [0, 1], \ N_x = N_y = 256, \text{ and the QTT tolerance is } 10^{-6}. \\
\end{align*} \]

We compare the time stepping solution scheme with the block approach. The number of time steps varies \( 2^8 \) to \( 2^{16} \), the CPU times/sec.

<table>
<thead>
<tr>
<th>( N_t )</th>
<th>Block solution</th>
<th>Time stepping</th>
</tr>
</thead>
<tbody>
<tr>
<td>( 2^8 )</td>
<td>CPU time</td>
<td>( | \Delta u(1) - f | )</td>
</tr>
<tr>
<td>( 76.96 )</td>
<td>1.53e+03</td>
<td>37.17</td>
</tr>
<tr>
<td>( 2^{10} )</td>
<td>83.23</td>
<td>7.34e-03</td>
</tr>
<tr>
<td>( 2^{12} )</td>
<td>69.32</td>
<td>1.44e-04</td>
</tr>
<tr>
<td>( 2^{14} )</td>
<td>60.40</td>
<td>3.67e-05</td>
</tr>
<tr>
<td>( 2^{16} )</td>
<td>61.37</td>
<td>5.49e-05</td>
</tr>
</tbody>
</table>

Notice: the solution time even decreases with the number of time steps in the block algorithm since the smaller the time step, the smoother the solution is. The QTT-rank is stable with respect to the number of time steps, and manifests also a slight decrease due to the improving smoothness of the solution. It demonstrates the advantages of the logarithmic scaling of the block scheme, especially if we have to choose extremely small time steps.

The Fokker-Planck equation

Real-time evolution. The Fokker-Planck equation

\[ \frac{d\psi}{dt} = -A\psi, \quad \psi(0) = \psi_0; \quad A\psi = -\varepsilon \Delta \psi + \text{div}(\psi v), \]

the probability density \( \psi : \mathbb{R}^d \rightarrow \mathbb{R} \), and \( v : \mathbb{R}^d \rightarrow \mathbb{R}^d \) is a given velocity field.

Time propagation scheme with tensor truncation

\[ \psi_{k+1} = T_\varepsilon (S \psi_k), \quad \psi_k \approx \psi(t_k), \quad t_k = \tau k. \]

The time-propagator \( S \):

\[ S = (I + \tau A)^{-1} \] (implicit Euler),

\[ S = (I + \frac{\tau}{2} A)^{-1} (I - \frac{\tau}{2} A) \] (Crank-Nicolson).

The time evolution converges to the null-space of \( A \), \( \psi_k \rightarrow \psi_* \),

\[ A\psi_* = 0, \quad \int \psi_* dx_1 \ldots dx_d = 1. \]

\( \psi_* \) is normalized probability density.
The *dumbbell model* discretized on large grids.

\[ \mathbf{v} = K \mathbf{q} + \nabla \varphi, \]

\[ K = \beta \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \mathbf{q} = \begin{pmatrix} q_1 \\ q_2 \\ q_3 \end{pmatrix} \]

The potential energy \( \varphi \) is given as

\[ \varphi = \frac{1}{2} (q_1^2 + q_2^2 + q_3^2) + \frac{1}{2} \frac{z}{p^3} e^{-\frac{(q_1^2 + q_2^2 + q_3^2)}{2p^2}}. \]

The following functional of the solution is of interest:

\[ \tau(t) = \int \psi(t) (\mathbf{q} \otimes \nabla \varphi) \, dq. \]

In particular, we test

\[ \eta(t) = -\frac{\tau_{12}}{\beta}, \quad \Psi(t) = -\frac{\tau_{11} + \tau_{22}}{\beta}. \]

### Numerics for the Fokker-Planck equation: time stepping vs. block solver

The *dumbbell model*: Complexity vs. \( N_t \) and \( N_x \).

**Figure:** TT-solution time vs. \( \tau \), \( N_x = 2^{d_x}, N_t = 2^{d_t} \),

Time \( \sim O(r^2 N_t N_x) \).

**Figure:** Block QTT-solution time vs. \( d_t, d_x \), \( O(r^2 \log N_t \log N_x) \),

\[ r = O(\log N_x) = O(d_x). \]

[Dolgov, BNK, Oseledets 'SISC-11]
▶ **QTT-Tucker for chemical master equation:** Species $S_1, \ldots, S_d$ react in $M$ channels.

The vector of concentration $x = (x_1, \ldots, x_d)$, $x_i \in \{0, \ldots, N_i - 1\}$, $i = 1, \ldots, d$.

The propensity function $w^m(x), m = 1, \ldots, M$.

The stoichiometric vector $z^m \in \mathbb{Z}^d$.

\[
J^z = \begin{bmatrix}
0 & \cdots & 1 \\
\vdots & \cdots & \vdots \\
0 & \cdots & 1 \\
\end{bmatrix} \quad \text{← row } N - z, \quad \text{if } z \geq 0; \quad J^z = (J^{-z})^\top, \quad \text{if } z < 0.
\]

CME is a deterministic difference equation on the joint probability density $P(x, t)$:

\[
\frac{dP(t)}{dt} = \sum_{m=1}^{M} (J^{z^m} - J^0) \text{diag}(w^m)P(t), \quad P(t) \in \mathbb{R}_{+}^{\prod_{i=1}^{d} N_i},
\]

\[
w^m = \{w^m(x)\} \quad \text{and} \quad P(t) = \{P(x, t)\}, \quad x \in \bigotimes_{i=1}^{d} \{0, \ldots, N_i - 1\}.
\]

**Long-time dynamics: CME for the signaling cascade, $d = 20$**

[Dolgov, BNK, NLAA ’13]

**Figure: Cascade signaling network**

- $d = 20$, $M = 40$;
- for $m = 1$: $w^m(x) = 0.7$, $z^m = -\delta_m$: generation of the first protein;
- for $m = 2, \ldots, 20$: $w^m(x) = \frac{x_{m-1}}{5 + x_{m-1}}$, $z^m = -\delta_m$: succeeding creation reactions;
- for $m = 21, \ldots, 40$: $w^m(x) = 0.07 \cdot x_{m-20}$, $z^m = \delta_{m-20}$: destruction reactions.
- $N_i = 63$.

$\delta_m$ is the $m$-th identity vector.

Problem size $N = 64^{20}$. 
Convergence history, $O(\log N_t)$ CPU time

- Two-level $t$-stepping: numbers of time steps $N_t$ in each interval $[(p - 1)T_0, pT_0]$,
- the time interval widths $T_0$ (coarse step): $N_T = T / T_0$.
- logarithmic complexity in $N_t$

![Figure: Mean concentrations](image1.png)

![Figure: Closeness to the kernel](image2.png)

![Figure: CPU time (sec.)](image3.png)

Figure: Mean concentrations $\langle x_i \rangle(t)$.

Figure: Closeness to the kernel $\|\mathcal{AP}\|/\|P\|(t)$.

Figure: CPU time (sec.) vs. $\log_2(N_t)$, $T_0 = 15$.

Boris N. Khoromskij Linz, RICAM, Research Semester, WS2, 10.11.2016

Tensor approximation of parabolic PDEs

Summary: Rank-structured tensor methods for PDEs in $\mathbb{R}^d$ and beyond

- Tensor MLA, $O(d \log N)$-approximation in QTT tensor format.
- New RS tensor formats: approximation tool for complicated data $(\pm)$.
- Super-fast computation of oscillatory integrals in $O(d \log N)$ cost $(\pm)$.
- QTT approximation of elliptic PDEs with "defected" periodic coefficients $(\pm)$.
- Low-rank IGA analysis for $d = 2, 3$ $(\pm)$.
- Multidimensional dynamics by QTT-AMEn solver for global $(x, t)$-system $(\mp)$.
- Time dependent Fokker-Planck and master eqn. in $d + 1$ $(\pm)$.
- High-dimensional horizons: log-scaling in time and space discretizations

This talk is based on the joint works:


[Dolgov, BNK '13], [Dolgov, BNK, Oseledec's '12]

[Mantzaflaris, Jüttler, BNK, Langer '15-'16], LNCS 9213, 2015; MPI preprint, 2016.

[BNK, Repin '15], RJNAMM 2015.

[BNK, Sauter, Veit], CMAM, '11-'15.

Thank you for your attention!