Range-separated tensor format for computation of electrostatics in large bio-molecules

Boris N. Khoromskij

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Based on joint works with B. Benner, V. Khoromskaia, C. Kweyu, M. Stein

Max-Planck-Institute for Mathematics in the Sciences, Leipzig, Germany

Outline of the talk

Basics of tensor numerical methods

- **Bridging multilinear algebra and rank-structured approximation of d-variate functions and operators $\Rightarrow$ tensor numerical methods**
- Low-rank sinc-approxim. of functions and operators [Gavrilyuk, Hackbusch, BNK '03-'08]
- Tensor formats extend rank-R matrices:

$$d = 2: \quad V = \sum_{k=1}^{R} \mathbf{u}_k \mathbf{v}_k^T \equiv G_1 G_2^T \equiv UDV^T \in \mathbb{R}^{m \times n}.$$

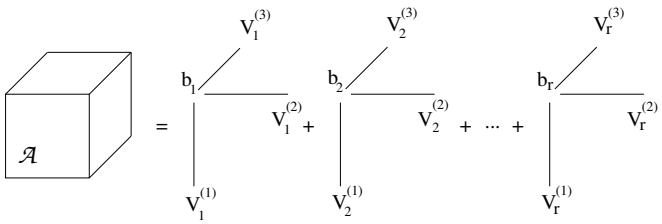
– Canonical (**CP**) tensors (multidimensional rank-R representation) [Hitchcock '27].
– **Orthogonal Tucker** decomposition (d-dimensional truncated SVD) [Tucker '66]
– Matrix product states (**MPS**) factorization [S. White '92 et al.]
– Hierarchical dimension splitting [BNK '06]
– Tensor train (**TT**) [Oseledets, Tyrtyshnikov '09]
– Hierarchical Tucker (**HT**) [Hackbusch, Kühn '09]
– **QTT** tensor approximation of discretized functions [BNK '09]; matrices [Oseledets '09]
– Range separated (**RS**) tensor format for approximating functions in $\mathbb{R}^d$ with multiple singularities [Benner, Khoromskaia, BNK '16]

Rank-R canonical (CP) tensor format

Def. Canonical (CP) R-term representation in $\mathbb{V}_{\mathbf{n}}$: $\mathbf{V} \in \mathcal{C}_R(\mathbb{V}_{\mathbf{n}})$,

$$\mathbf{V} = \sum_{k=1}^{R} \mathbf{v}_k^{(1)} \otimes \ldots \otimes \mathbf{v}_k^{(d)}, \quad \mathbf{v}_k^{(\ell)} \in \mathbb{R}^{n_\ell}.$$

- Advantages: Storage $= dRN$, simple multilinear algebra, analytic (sinc) methods of approximation
- Limitations: Hard for numerical approximation.



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

- **Rank reduction in the CP format via Reduced HOSVD**:

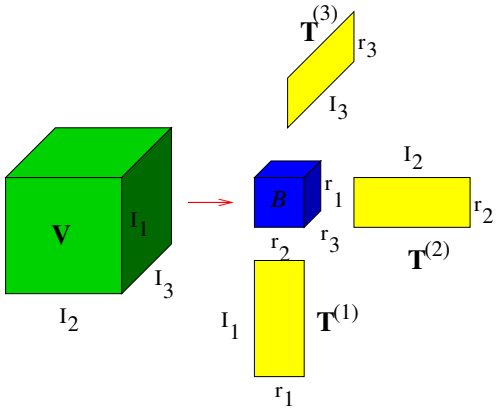
(A) Canonical $\mapsto$ Tucker, (B) the small Tucker core $\mapsto$ CP [BNK, Khoromskaia, SISC '08].

Orthogonal Tucker decomposition

Def. Rank $\mathbf{r} = (r_1, \ldots, r_d)$ **Tucker tensors:** $\mathbf{V} \in \bigotimes_{\ell=1}^{d} T_\ell \subset \mathbb{V}_{\mathbf{n}}$

$$\mathbf{V} = \sum_{k_1,\ldots,k_d=1}^{\mathbf{r}} b_{k_1\ldots k_d} \mathbf{v}_{k_1}^{(1)} \otimes \ldots \otimes \mathbf{v}_{k_d}^{(d)} = \mathbf{B} \times V^{(1)} \times \cdots \times V^{(1)}, \quad T_\ell = span\{\mathbf{v}_{k_\ell}^{(\ell)}\}_{k_\ell=1}^{r_\ell} \subset \mathbb{R}^{n_\ell}$$

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

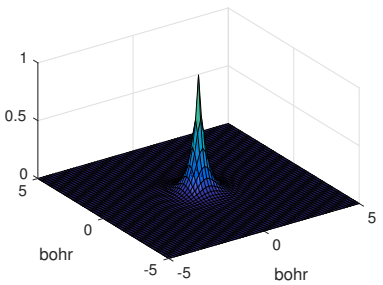


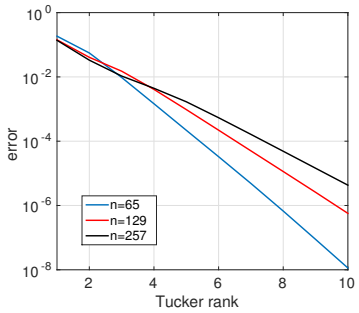
- **Reducing the Tucker rank by higher order SVD (HOSVD)** [De Lathauwer et.al., 2000]

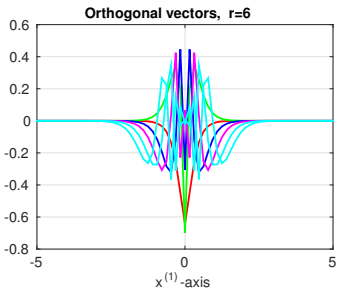
Tucker tensor decomposition of function related tensors

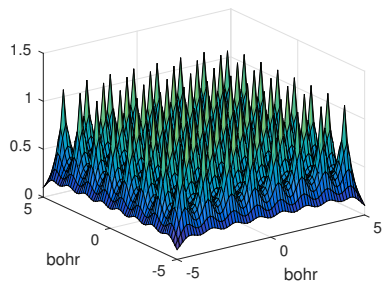
[BNK, '06], [BNK, V. Khoromskaia '07]

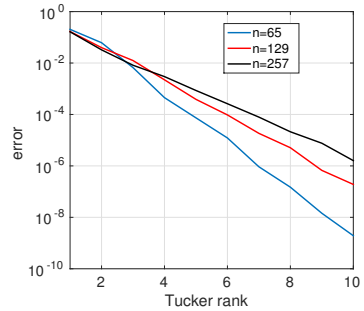
Example: Slater function $f(x) = e^{-\alpha\|x\|}$, $x \in \mathbb{R}^3$, $E_{FN} = \frac{\|A_0 - A_{(r)}\|}{\|A_0\|}$

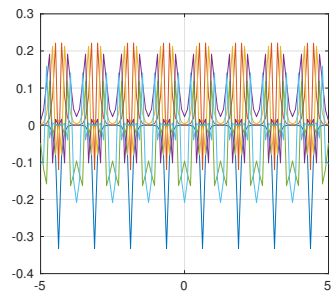












Multi-centered $8 \times 8 \times 8$ Slater, multigrid Tucker: $O(n^3)$ instead of $O(n^4)$.

Grid-based tensor methods for (post) Hartree-Fock calculus

The Hartree-Fock (HF) nonlinear integral-differential eigenvalue problem (EVP)

$$\mathcal{F}\varphi_i(x) \equiv (-\frac{1}{2}\Delta + V_c + V_H - \mathcal{K})\varphi_i(x) = \lambda_i \varphi_i(x), \qquad i = 1, ..., N_{orb}.$$

The Fock operator $\mathcal{F}$ depends on the density matrix $\tau(x,y) = 2\sum_{i=1}^{N_{orb}} \varphi_i(x)\varphi_i(y)$,

$$\mathcal{F}\varphi := [-\frac{1}{2}\Delta - \sum_{\nu=1}^{M_0} \frac{Z_\nu}{\|x - a_\nu\|} + \int_{\mathbb{R}^3} \frac{\tau(y,y)}{\|x-y\|}\, dy]\varphi - \frac{1}{2}\int_{\mathbb{R}^3} \frac{\tau(x,y)}{\|x-y\|}\, \varphi(y)dy.$$

Given the atomic orbital (AO) basis $\{g_\mu(x)\}$, $\mu = 1, ..., N_b$.
The 4-order two-electron integrals (TEI) tensor

$$b_{\mu\nu\kappa\lambda} = \int_{\mathbb{R}^3\times\mathbb{R}^3} \frac{g_\mu(x)g_\nu(x)g_\kappa(y)g_\lambda(y)}{\|x-y\|}\, dxdy.$$

Important case (post-HF) : the molecular orbital (MO) basis $\{\varphi_i(x)\}$, $i = 1, ..., N_{orb}$.

Numerical challenges: Large TEI tensor of size N_b^4; 3D multiple convolutions; nuclear cusps; high accuracy; strongly nonlinear eigenvalue problem; excitation energies; DOS for optical spectra of molecules.

Piece of history: tensor methods in HF and post-HF calculations

- Grid-based tensor methods for HF equation.
  [Khoromskaia, BNK, '09 - '15], [BNK, Khoromskaia, Flad, '11]
- Rank approximation of the two-electron integrals (TEI)
  [Khoromskaia, BNK, Schneider, SISC '13], [Khoromskaia, BNK, CPC '14]
- $L \times L \times L$ lattice sum of electrostatic potentials, $1/\|x\|$, in $O(L)$ cost.
  [Khoromskaia, BNK, CPC '14, NLLA '16]
- Post-HF: excitation energies via rank-structured approx. to BSE system matrix; density of states
  [Benner, Khoromskaia, BNK, MolPhys '15], [Benner, Dolgov, Khoromskaia, BNK, JCP '16], [Benner, Khoromskaia, BNK, Yang, '17]
- Range-separated (RS) tensor format for long range multi-particle interactions
  [Benner, Khoromskaia, BNK, SISC '18]
- B. Khoromskij. Tensor numerical methods in scientific computing. De Gruyter, Berlin, 2018.
- V. Khoromskaia, B. Khoromskij. Tensor numerical methods in electronic structure calculations. De Gruyter, Berlin, 2018.

I. CP tensor approx. of RB funct. $p(\|x\|)$, the Newton kernel $p(\|x\|) = \frac{1}{\|x\|}$

[Stenger '93], [Braess '95], [Gavrilyuk, Hackbusch, BNK '05], [Bertoglio, BNK '08]

The Laplace-Gauss transform for the analytic radial basis (RB) functions $p(\|x\|)$

$$p(z) = \frac{2}{\sqrt{\pi}} \int_{\mathbb{R}_+} \tilde{p}(t) e^{-t^2 z^2} dt \approx \sum_{k=-M}^{M} a_k e^{-t_k^2 \|x\|^2} = \sum_{k=-M}^{M} a_k \prod_{\ell=1}^{3} e^{-t_k^2 x_\ell^2}.$$

Sinc-quadrature approximation converges exponentially fast in M ($0 < h \le \|x\|$):

$$\left| \frac{1}{\|x\|} - \sum_{k=-M}^{M} a_k \prod_{\ell=1}^{3} e^{-t_k^2 x_\ell^2} \right| \le \frac{C}{h} e^{-\beta\sqrt{M}}, \quad \text{with some } C, \beta > 0,$$

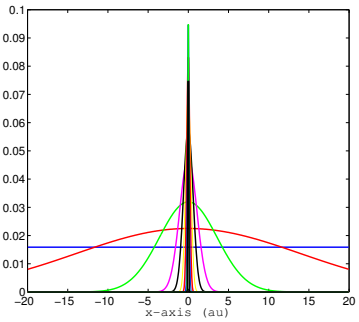
where the quadrature points and weights are given by ($a(t_k) = \frac{2}{\sqrt{\pi}}$)

$$t_k = k\mathfrak{h}_M, \quad a_k = a(t_k)\mathfrak{h}_M, \quad \mathfrak{h}_M = C_0 \log(M)/M, \quad C_0 > 0.$$

$$\mathbf{P} := [p_{\mathbf{i}}] \in \mathbb{R}^{n\times n\times n}, \quad p_{\mathbf{i}} = \int_{\mathbb{R}^3} \frac{\psi_{\mathbf{i}}(\mathbf{x})}{\|\mathbf{x}\|} d\mathbf{x}, \quad \psi_{\mathbf{i}}(\mathbf{x}) = \prod_{\ell=1}^{d} \psi_{i_\ell}^{(\ell)}(x_\ell), \quad i_\ell = 1, ..., n, \ \ell = 1, 2, d.$$

Canonical tensor approximation of the Newton kernel

$$\mathbf{P}_N = \sum_{q=1}^{R_N} \mathbf{p}_q^{(1)} \otimes \mathbf{p}_q^{(2)} \otimes \mathbf{p}_q^{(3)}, \quad \mathbf{p}_q^{(\ell)} \in \mathbb{R}^{n_\ell}, \quad \ell = 1,\ 2,\ 3.$$



Canonical vectors $\mathbf{p}_q^{(1)}$ of the symmetric tensor $\mathbf{P}_N$.

grid size n^3	8192^3	16384^3	32768^3	65536^3	131072^3
Time (s)	1	2	8	43	198
Canonical rank R	34	36	38	40	42
Compression rate	$2 \cdot 10^6$	$7 \cdot 10^6$	$2 \cdot 10^7$	$1 \cdot 10^8$	$4 \cdot 10^8$

CPU times (Matlab) to generate a canonical tensor $\mathbf{P}_N$ for the Newton kernel, $\varepsilon = 10^{-6}$.

Classical methods for summation of long-range potentials

Computing sums of long range electrostatic potentials on large $L \times L \times L$ lattices,

$$V_c(x) = \sum_{a=1}^{L^3} \frac{Z_a}{\|x - x_a\|}, \; x \in \mathbb{R}^3, \quad \text{and} \quad E_{nuc} = \sum_{a=1}^{L^3} \sum_{m<a}^{L^3} \frac{Z_a Z_m}{\|x_a - x_m\|}. \tag{1}$$

Ewald summation, [Ewald, 1927], fast multipole method [Greengard, Rochlin '87].
A sum of potentials on a $L \times L \times L$ lattice,

$$v_{c_L}(x) = \sum_{k_1,k_2,k_3=1}^{L} \frac{Z}{\|x - a(k_1,k_2,k_3)\|}, \quad x \in \Omega_L = \bigcup_{k_1,k_2,k_3=1}^{L} \Omega_{\mathbf{k}} \in \mathbb{R}^3,$$

Ewald summation is based on a local-global decomposition of the Newton kernel

$$\frac{1}{r} = \frac{\tau(r)}{r} + \frac{1-\tau(r)}{r}, \quad r = \|x\|,$$

where the choice of cutoff function τ is the complementary error function

$$\tau(r) = \mathrm{erfc}(r) := \frac{2}{\sqrt{\pi}} \int_r^\infty \exp(-t^2) dt.$$

$\Rightarrow O(L^3)$ instead of $O(L^6)$ for direct sum (1).

II. Lattice sum of potentials by tensor decomposition: $O(L)$ versus $O(L^3)$

[Khoromskaia & Khoromskij CPC'14]
We consider the sum of potentials defined on the domain Ω_L,

$$v_{c_L}(x) = \sum_{k_1,k_2,k_3=1}^{L} \frac{Z}{\|x - b\mathbf{k}\|}, \quad x \in \Omega_L. \tag{2}$$

Then the projected tensor representation of $v_{c_L}(x)$ takes the form (omitting factor Z)

$$\mathbf{P}_{c_L} = \sum_{k_1,k_2,k_3=1}^{L} \mathcal{W}_{\nu(\mathbf{k})} \mathbf{P}_N = \sum_{k_1,k_2,k_3=1}^{L} \sum_{q=1}^{R} \mathcal{W}_{(\mathbf{k})} (\mathbf{p}_q^{(1)} \otimes \mathbf{p}_q^{(2)} \otimes \mathbf{p}_q^{(3)}) \in \mathbb{R}^{n_L \times n_L \times n_L},$$

where the 3D shift vector is defined by $\mathbf{k} \in \mathbb{Z}^{L \times L \times L}$. $\mathcal{W}_{(\mathbf{k})} = \mathcal{W}^{(1)}_{(k_1)} \otimes \mathcal{W}^{(2)}_{(k_2)} \otimes \mathcal{W}^{(3)}_{(k_3)}$.

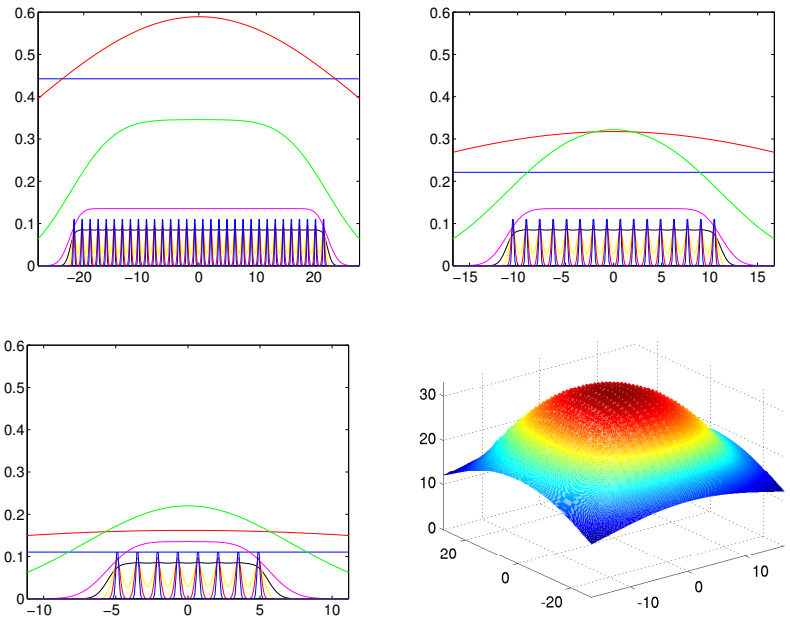
Theorem

Given rank-R canonical tensor $\mathbf{P}_N$, the sum of electrostatic potentials $v_{c_L}(x)$, $x \in \Omega_L$, of the lattice with L^3 charges is presented by the canon. tensor $\mathbf{P}_{c_L}$ of the same rank R,

$$\mathbf{P}_{c_L} = \sum_{q=1}^{R} \Big(\sum_{k_1=1}^{L} \mathcal{W}_{(k_1)} \mathbf{p}_q^{(1)} \Big) \otimes \Big(\sum_{k_2=1}^{L} \mathcal{W}_{(k_2)} \mathbf{p}_q^{(2)} \Big) \otimes \Big(\sum_{k_3=1}^{L} \mathcal{W}_{(k_3)} \mathbf{p}_q^{(3)} \Big). \tag{3}$$

Sums of potentials by assembled canonical/Tucker vectors

Assembled vectors of the canonical tensor representing a sum of electrost. potentials on a lattice (abs. accuracy 10^{-14}).

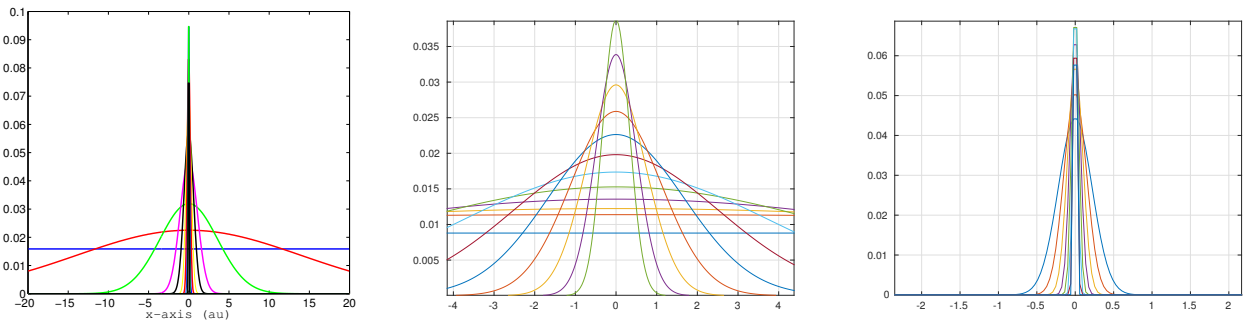


Assembled vectors in x-, y-, z for a cluster of $32 \times 16 \times 8$ Hydrogen atoms (4096).

III. Range separated CP tensor approx. of the Newton kernel $\frac{1}{\|x\|}$ on a grid

$$\mathbf{P} \approx \mathbf{P}_R = \sum_{k=-M}^{M} a_k \bigotimes_{\ell=1}^{3} \mathbf{b}^{(\ell)}(t_k) = \sum_{q=1}^{R} \mathbf{p}_q^{(1)} \otimes \mathbf{p}_q^{(2)} \otimes \mathbf{p}_q^{(3)} \in \mathbb{R}^{n\times n\times n}$$

$$R \leq 2M + 1 \approx C|\log \varepsilon|$$



IV. Range-separated (RS) tensor format for approximating funct. with multiple cusps

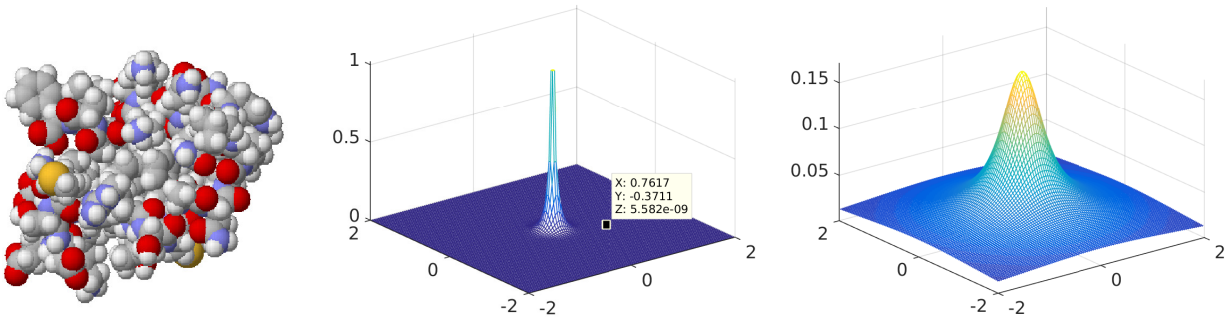


Figure: Villin protein (left). Short- and long-range parts of the reference Newton kernel $1/\|x\|$.

[Benner, Khoromskaia, BNK '16]

Definition

(RS-canonical tensors). The RS-canonical format defines the class of d-tensors $\mathbf{A} \in \mathbb{R}^{n_1 \times \cdots \times n_d}$, represented by a sum of a rank-R CP tensor $\mathbf{U}$ and a cumulated CP tensor generated by localized $\mathbf{U}_0$, s.t.

$$\mathrm{rank}(\mathbf{U}_\nu) = \mathrm{rank}(\mathbf{U}_0) \le R_0, \quad \mathbf{U}_\nu = \mathrm{Replica}(\mathbf{U}_0),$$

$$\mathbf{A} = \sum_{k=1}^{R} \xi_k \mathbf{u}_k^{(1)} \otimes \cdots \otimes \mathbf{u}_k^{(d)} + \sum_{\nu=1}^{N_0} c_\nu \mathbf{U}_\nu, \quad \text{with} \quad \mathrm{diam}(\mathrm{supp}\mathbf{U}_\nu) \le 2\gamma.$$

RS canonical format: beneficial properties (similar: RS-Tucker, RS-TT)

Theorem

[Benner, Khoromskaia, BNK '16] *The storage size for RS-canonical tensor is estimated by*

$$stor(\mathbf{A}) \le dRn + (d+1)N_0 + R_0\gamma.$$

Each entry of an RS-CP tensor can be calculated at $O(dR + 2d\gamma R_0)$ cost.
ε-rank $\mathbf{r}_0$ of the Tucker approximation to the long-range CP tensor $\mathbf{U}$ is bounded by

$$|\mathbf{r}_0| := rank_{Tuck}(\mathbf{U}) \le C\, b\, \log^{3/2}(|\log(\varepsilon/N_0)|).$$

Corollary

The following operations on RS canonical/Tucker tensors can be realized efficiently:
(a) construction of functional interpolants in $\mathbb{R}^d$ via radial basis functions.
(b) summation of many-particle interaction potentials meshed up on a fine grid in $\mathbb{R}^d$.
(c) computation of interaction energy, gradients and forces for many-particle system.

▶ RS-CP tensor $\mathbf{A} \in \mathbb{R}^{n_1 \times \cdots \times n_d}$ is uniquely defined by the following parametrization: rank-R CP tensor $\mathbf{U}$, the rank-R_0 reference CP tensor $\mathbf{U}_0$ with mode-size $\le 2\gamma$, list $\mathcal{J}$ of the coordinates and weights of N_0 particles in $\mathbb{R}^d$.

Bounds on tensor rank in Theorem: analysis in the frequency domain

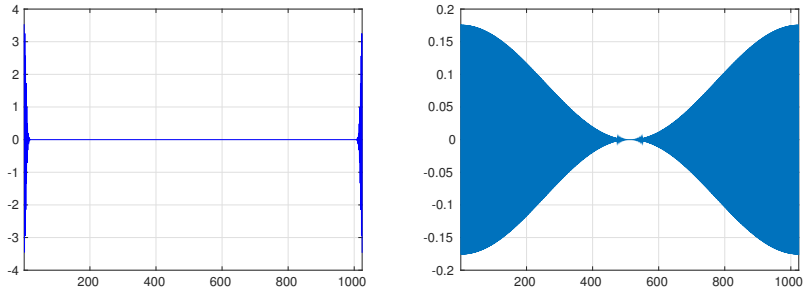


Figure: *Fourier coef. of the long- (left) and short-range (right) discrete Gaussians*, $n = 1024$.

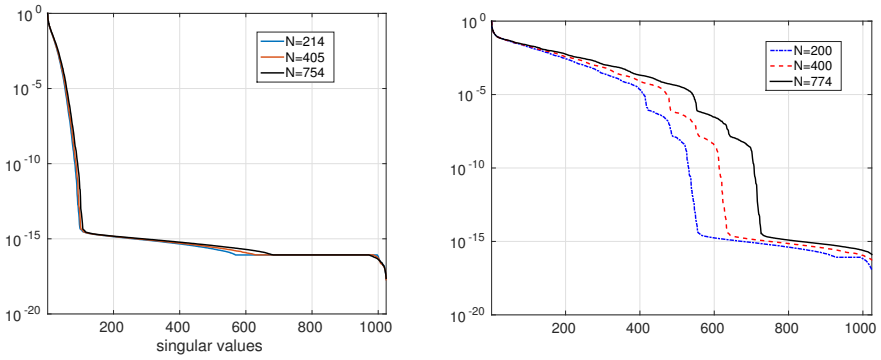


Figure: *Mode-1 singular values of side matrices for the full sum and long-range part* $\mathbf{P}_l$ *vs.* $N_{\mathbf{0}}$, $R_l = 12$.

RS canonical format: how to split the short and long range parts

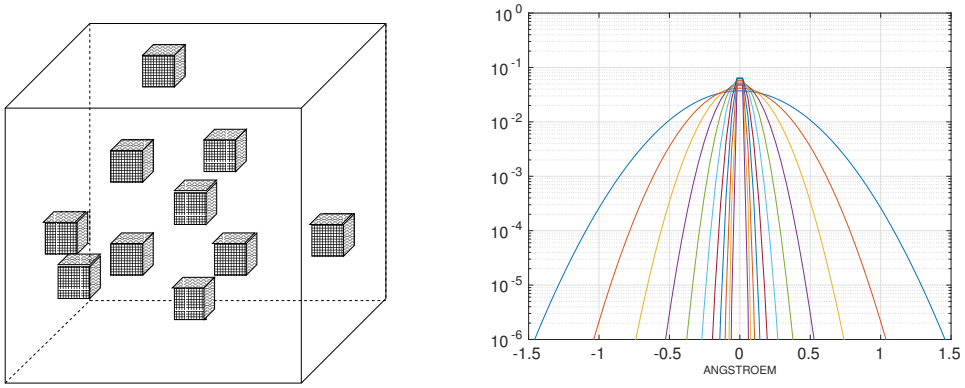


Figure: *Effective supports of the CCT (left); short-range canonical vectors for* $k = 1, \ldots, 11$ *on log-scale.*

N_0 / R_{long}	8	9	10	11	12	13
200	10,10,11	13,12,12	18,15,16	23,19,21	32,24,27	42,30,34
400	11,10,11	14,13,14	19,16,20	26,21,26	35,27,36	47,34,47
782	11,11,12	15,14,15	20,18,20	28,26,27	39,35,37	52,46,50

Table: *Tucker ranks* $\mathbf{r} = (r_{\mathbf{1}}, r_{\mathbf{2}}, r_{\mathbf{3}})$ *for the long-range part of* $N_{\mathbf{0}}$*-nuclei electrostatic potential,* $\epsilon = 10^{-\mathbf{6}}$.

- The classes of RS-Tucker and RS-TT tensors are defined completely similar.

RS format applies to a general class of RB functions, Green's kernels

RS-tensor approximation applies to a wide class of long-range RB funct. $p(\|x\|)$ in $\mathbb{R}^3$:

$$\text{Slater function:} \quad p(\|x\|) = \exp(-\lambda\|x\|), \quad \lambda > 0,$$

$$\text{Yukawa kernel:} \quad p(\|x\|) = \frac{\exp(-\lambda\|x\|)}{\|x\|}, \quad \lambda > 0,$$

$$\text{Lennard-Jones potential:} \quad p(\|x\|) = 4\epsilon \left[\left(\frac{\sigma}{\|x\|}\right)^{12} - \left(\frac{\sigma}{\|x\|}\right)^{6} \right],$$

The simplified version of the Lennard-Jones potential, the Buckingham function

$$\text{Buckingham potential:} \quad p(\|x\|) = 4\epsilon \left[e^{\|x\|/r_0} - \left(\frac{\sigma}{\|x\|}\right)^{6} \right].$$

The electrostatic dipole-dipole potential energy (Van der Waals forces)

$$\text{Dipole-dipole interaction energy:} \quad p(\|x\|) = \frac{C_0}{\|x\|^3}.$$

V. The Poisson-Boltzmann eqn. for electrostatic potential of a bio-molecule

- The linearized Poisson-Boltzmann (PB) equation [Lu, Zhou, Holst, McCammon '08]

$$-\nabla\cdot(\epsilon\nabla u) + \kappa^2 u = \rho_f = \sum_{k=1}^{N} z_k \delta(\|x - x_k\|) \quad \text{in} \quad \Omega = \Omega_s \cup \Omega_m,$$

where u is the target electrostatic potential of a protein, ρ_f is the scaled singular charge distribution supported at points $x_k \in \Omega_m$, $\kappa = 0, \epsilon = 1$ in Ω_m.
The interface conditions on the interior boundary $\Gamma = \partial\Omega_m$: $[u] = 0$, $\left[\epsilon \frac{\partial u}{\partial n}\right] = 0$ on Γ.

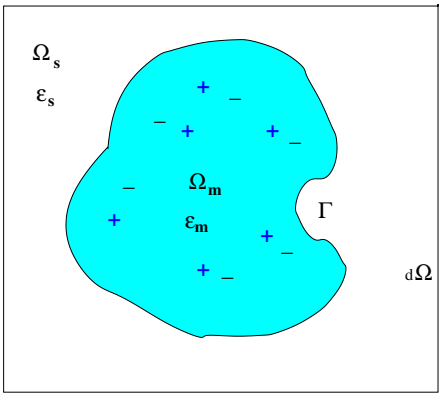


Figure: Computational domain for PBE: Solute (molecule) region Ω_m, solvent Ω_s.

[Benner, Khoromskaia, BNK, C. Kweyu, M. Stein, '18]

- Idea: RS splitting of the Dirac delta $\Rightarrow$ regularize the right-hand side ρ_f, [BNK '18]

VI. RS splitting of the Dirac delta

A sum of the short- and long-range tensors,

$$\frac{1}{\|x\|} \rightsquigarrow \mathbf{P}_R = \mathbf{P}_{R_s} + \mathbf{P}_{R_l} \in \mathbb{R}^{n\times n\times n},$$

$$\mathbf{P}_{R_s} = \sum_{k=R_l+1}^{R} \mathbf{p}_k^{(1)} \otimes \mathbf{p}_k^{(2)} \otimes \mathbf{p}_k^{(3)}, \quad \mathbf{P}_{R_l} = \sum_{k=1}^{R_l} \mathbf{p}_k^{(1)} \otimes \mathbf{p}_k^{(2)} \otimes \mathbf{p}_k^{(3)}. \tag{4}$$

Discretize the exact equation for the Newton potential,

$$-\Delta \frac{1}{\|x\|} = 4\pi\,\delta(x), \quad \frac{1}{\|x\|} = -4\pi\Delta^{-1}\delta(x)$$

by using the FEM Laplacian matrix A_Δ instead of Δ and via substitution of the canonical tensor decomposition $\mathbf{P}_R$ instead of $u(x) = \frac{1}{\|x\|}$.

- This leads to the grid representation of the discretized Dirac delta [BNK '18]

$$\delta(x) \rightsquigarrow \boldsymbol{\delta}_h := -\frac{1}{4\pi} A_\Delta \mathbf{P}_R,$$

to be applied in the frame work of our regularization scheme.

Long-range part in the Dirac delta

3D finite difference Laplacian matrix A_Δ, on the uniform rectangular grid

$$A_\Delta = \Delta_1 \otimes I_2 \otimes I_3 + I_1 \otimes \Delta_2 \otimes I_3 + I_1 \otimes I_2 \otimes \Delta_3, \tag{5}$$

s.t. the Kronecker rank of A_Δ equals to 3.
$-\Delta_\ell = h_\ell^{-2}\mathrm{tridiag}\{1,-2,1\} \in \mathbb{R}^{n_\ell\times n_\ell}$, $\ell = 1,2,3$, denotes the discrete 1D Laplacian, I_ℓ, $\ell = 1,2,3$, is the identity matrix in the corresponding single dimension.

- Use the splitting of the discretized δ-function into short- and long-range components

$$\boldsymbol{\delta}_h = \boldsymbol{\delta}_s + \boldsymbol{\delta}_l, \tag{6}$$

where

$$\boldsymbol{\delta}_s := -\frac{1}{4\pi} A_\Delta \mathbf{P}_{R_s}, \quad \text{and} \quad \boldsymbol{\delta}_l := -\frac{1}{4\pi} A_\Delta \mathbf{P}_{R_l}. \tag{7}$$

- Simple example: the single charge.

The discrete Poisson eqn. for the long-range part $\mathbf{u}_l = \mathbf{P}_{R_l}$, in the full potential $u \approx \mathbf{P}_R = \mathbf{P}_{R_s} + \mathbf{P}_{R_l}$,

$$-A_\Delta \mathbf{u}_l = \boldsymbol{\delta}_l,$$

which can be solved by the favorable iterative method. Now

$$u \approx \mathbf{P}_R = \mathbf{P}_{R_s} + \mathbf{u}_l.$$

VII. Regularization of the PBE by RS splitting of the r.h.s.

- **Benefits:**
  - Jump conditions at the interface remain unchanged. Hence, the approach applies also to nonlinear PBE.
  - The long-range part in the RS tensor decomposition of the Dirac-delta [BNK '18] vanishes at the interface and, hence, the modified right-hand side generated by this long-range component remains localized in the "linear" solute region Ω_s.
  - A system of algebraic eqn. is solved for the smooth long-range (i.e., regularized) part of the collective potential discretized with controllable precision on a rather coarse grid. Solution is then added to the directly precomputed (avoiding solving PDE) low-rank tensor representation for the short-range part.
- Multi-atomic systems:

$$u \approx \mathbf{P}_{R_s} + \mathbf{u}_l; \qquad \rho_f = \sum_{k=1}^{N} z_k \delta(\|x - x_k\|) \approx \rho_{short} + \sum_{k=1}^{N} z_k \boldsymbol{\delta}_{l,k}$$

and solve regularized PBE with ($\mathbf{P}_{R_s}$ captures well singularities)

$$-\nabla \cdot (\epsilon \nabla \mathbf{u}_l) + \kappa^2 \mathbf{u}_l = \rho_{long}; \qquad \rho_{long} = \sum_{k=1}^{N} z_k \boldsymbol{\delta}_{l,k}.$$

ρ_{long} is represented in low-rank canonical (Tucker) format uniformly in molecular size N.

Numerics I

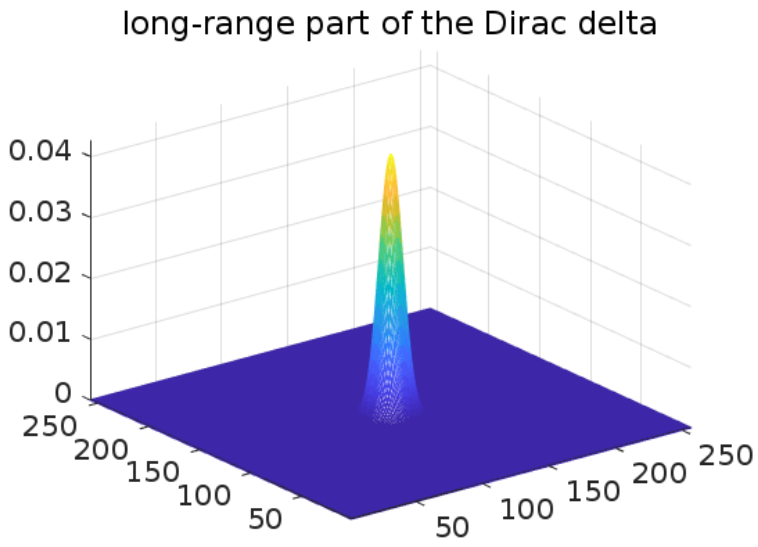


Figure: The long-range part of the Dirac delta δ_l on the $n^{\otimes 3}$ 3D grid, $n = 256$.

Numerics II

For the acetazolamide compound consisting of 18 atoms, determine the accuracy of the traditional PBE model vis a vis the PBE model modified by the RS tensor format. The modified PBE model provides highly accurate solutions as compared to those of the traditional PBE due to the accurate treatment of singularities by the RS-splitting of the Dirac delta.

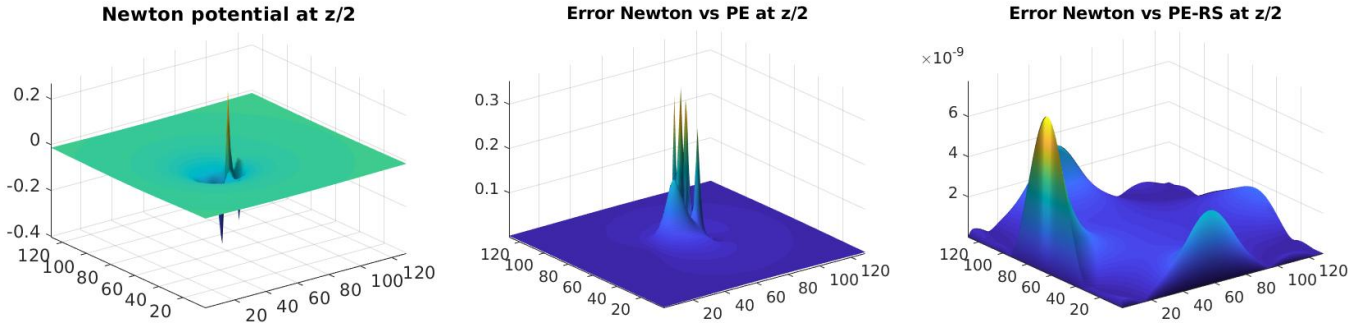


Figure: The free-space potential sums computed by the canonical tensor decomposition (left), the error of its computation on the same grid by using the classical PBE (middle) and by the modified PBE (right).

Summary: Tensor numerical methods for electrostatics in bio-molecules

- Efficient MLA in canonical, Tucker, TT formats, $O(d \log N)$-approximation by QTT tensors $(\pm)$.
- Tensor sums of interaction potentials on "defected" lattices $(+)$.
- New RS tensor formats: approximation tool for complicated data $(+)$.
- Low-rank tensor decomposition of interaction potentials with multiple singularities $(\pm)$.
- RS tensor splitting of the Dirac delte $(\pm)$.
- RS-based regularization scheme for the Poisson-Boltzmann equation $(\pm)$.

http://personal-homepages.mis.mpg.de/bokh

Thank you for your attention !