Tensor numerical modeling of the collective electrostatic potential in many-particle systems

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(joint talk with Boris Khoromskij)

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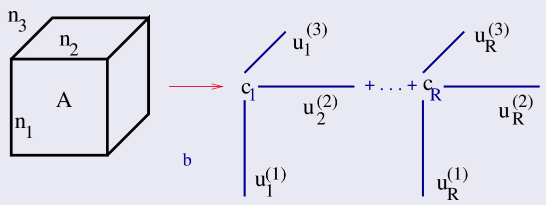
Outline of the lecture

1. What are tensor numerical methods?
   - Rank-structured representation of tensors
   - Bridging multilinear algebra and approximation theory
   - Algorithmic prerequisites to tensor methods
2. Tensor-based calculation of the 3D collective electrostatic potential
   - Grid-based low-rank representation of multidimensional potentials
   - Lattice sums by tensor approach : $O(L)$ instead of $O(L^3)$
   - Tensor sums on composite geometries
   - Interaction energy of charged particles on 3D lattices
3. Tensor-based collective electrostatic potentials in many-particle systems
   - Tensor-based range separation for a single Newton kernel
   - Summation of the long-range part of multiparticle potential
   - Range-separated tensor format for many-particle potentials

Rank-structured representation of tensors

$\mathbf{A} = [a_{i_1 \ldots i_d}] \in \mathbb{R}^{n_1 \times \ldots \times n_d}$, $(n_\ell = n)$ $N = n^d$ –"curse of dimensionality".

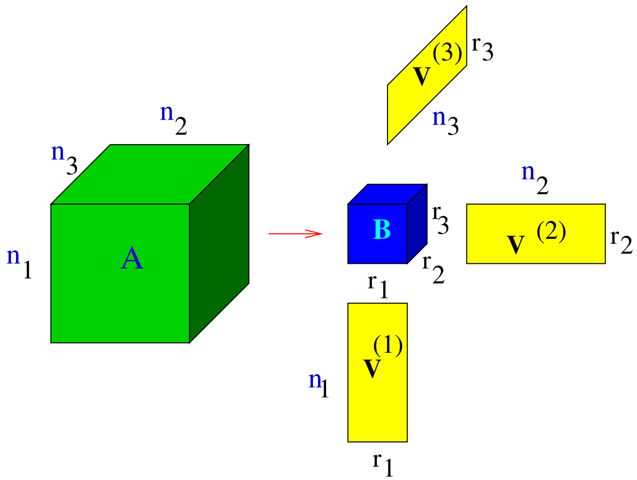
Canonical tensor format **[Hitchcock, 1927]**,



$$\mathbf{A} = \sum_{k=1}^{R} c_k \mathbf{u}_k^{(1)} \otimes \ldots \otimes \mathbf{u}_k^{(d)}$$

NP hard problem **[C J Hillar, LH Lim, 2013]** Storage $dRn \ll n^d$.

Tucker tensor format **[Tucker, 1966]**,



$$\mathbf{A}_{(\mathbf{r})} = \sum_{\nu_1=1}^{r_1} \ldots \sum_{\nu_d=1}^{r_d} \beta_{\nu_1,\ldots,\nu_d} \mathbf{v}_{\nu_1}^{(1)} \otimes \ldots \otimes \mathbf{v}_{\nu_d}^{(d)},$$

$$\boldsymbol{\beta} = [\beta_{\nu_1,\ldots,\nu_d}] \in \mathbb{R}^{r_1 \times \ldots \times r_d}$$

Storage $r^d + drn \ll n^d$

Bridging multilinear algebra and approximation theory

For tensor numerical methods:

Prerequisites from multilinear algebra:

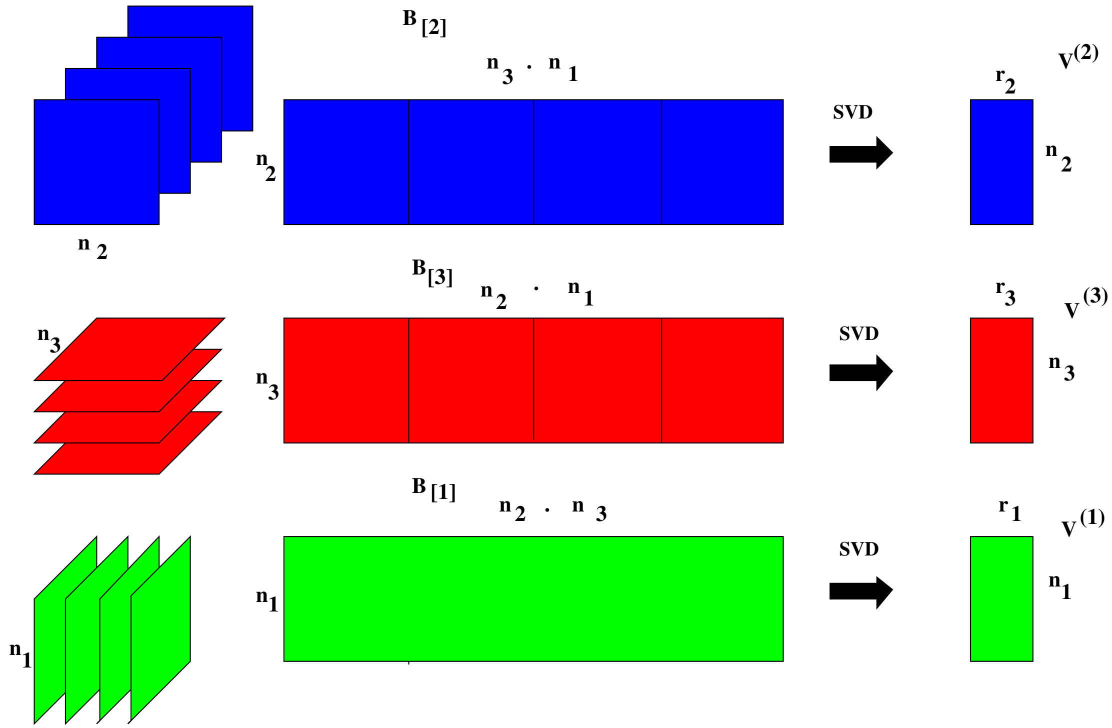
- Rank-structured representation of the multidimensional tensors by the canonical **[Hitchcock 1927]** and Tucker **[Tucker 1966]** tensor formats.
- Higher order SVD (HOSVD) for Tucker tensor decomposition (needs full size tensor, n^d), complexity $O(n^{d+1})$. **[De Lathauwer et al. 2000]**.
- Tensor is content independent: large ranks.

Prerequisites from the nonlinear approximation theory:

- Low-rank tensor-product decomposition of multivariate functions and operators based on the Sinc-quadrature method. **[Gavrilyuk, Hackbusch, Khoromskij 2003-2006]**.
- Constructive low-rank representation for Newton and Yukawa kernels via Laplace transform and sinc approximation. **[Bertolio, Khoromskij 2008]**
- Content of a tensor matters: logarithmic ranks, $r = O(\log n)$.

Tucker decomposition algorithm: Initial guess

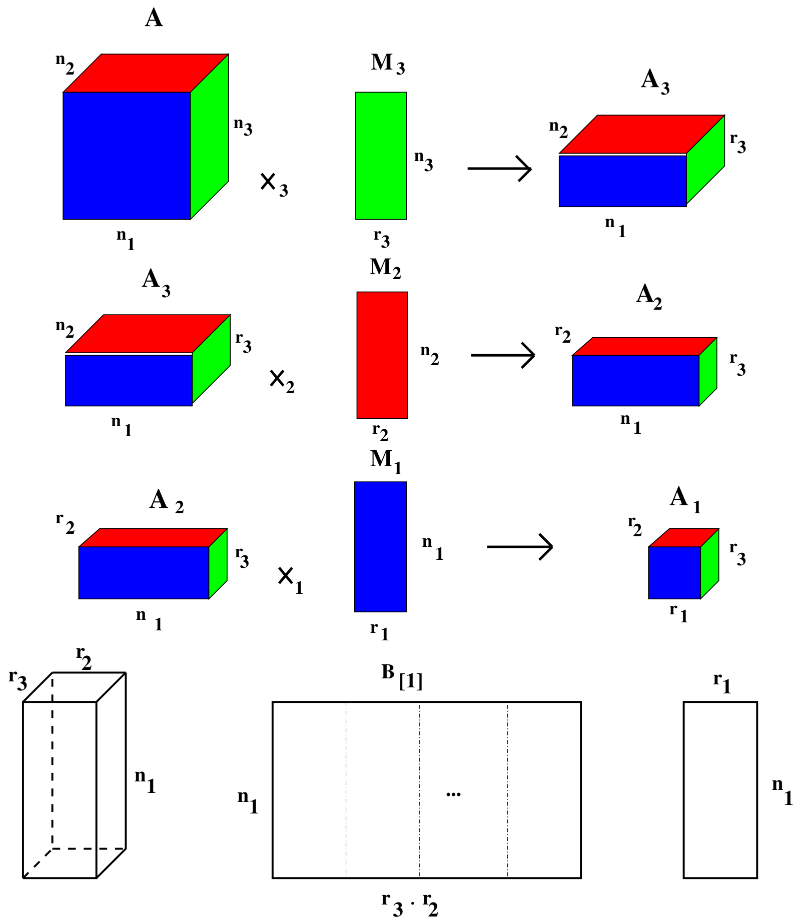
[De Lathauwer et al. 2000]
SVD of matrix unfoldings of a tensor and calculation of the initial guess for Tucker side matrices: SVD of the matrix of size of full tensor n^d needed!



Matlab commands: B= reshape(A,n1,n2*n3);
Or permute(A,[3,2,1]); B3= reshape(A,n3,n1*n2);

"Single-hole" tensor: Tucker ALS

[De Lathauwer et al. 2000] full size tensor n^d needed! Compute "single-hole" tensors for ALS by using contracted product of the initial 3D full-size tensor and orthogonal matrices $V^{(\ell)}, \ell = 1, 2, 3$ for all dimensions except one.



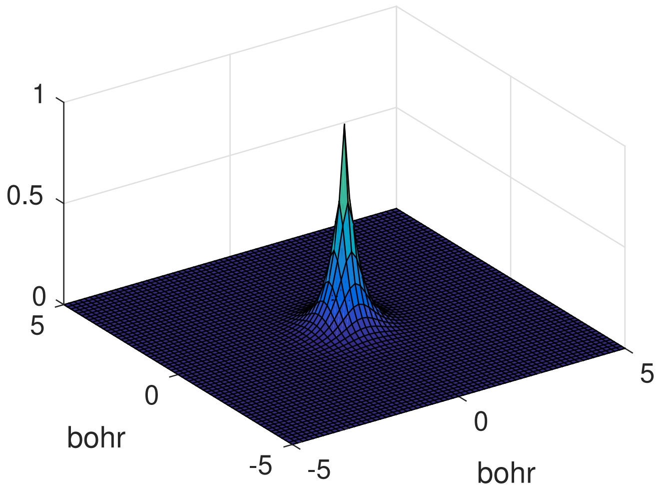
Tucker ALS: update $V^{(\ell)}$ by SVD of unfolding matrix of the "single hole tensor".

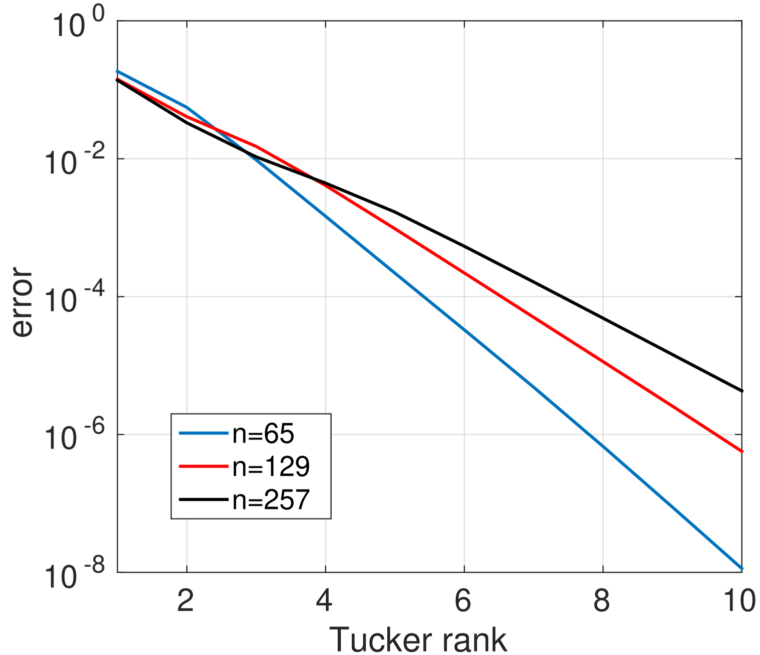
Prerequisites: functional Tucker approximation

For function related tensors the error of the Tucker decomposition **[Khoromskij 2006]**:

$$\|\mathbf{A}_{(r)} - \mathbf{A}_0\| \leq Ce^{-\alpha r},$$

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



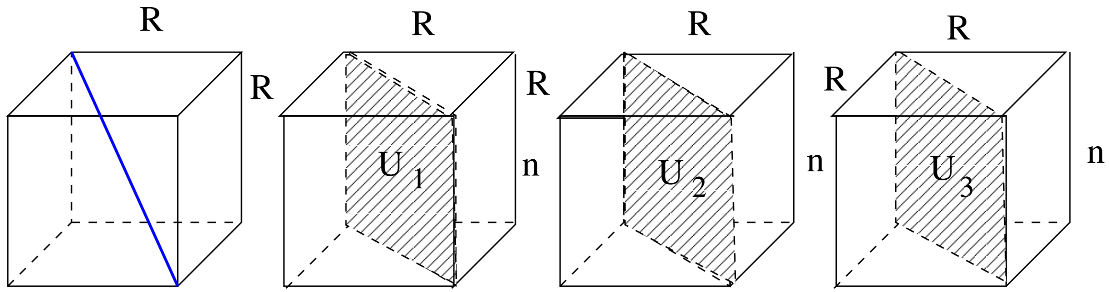


[Khoromskij, Khoromskaia, '07; SISC '09].

Multigrid Tucker: $O(n^3)$ instead of $O(n^4)$. SVD of full size tensor n^d not needed!

[Khoromskij & Khoromskaia '08]

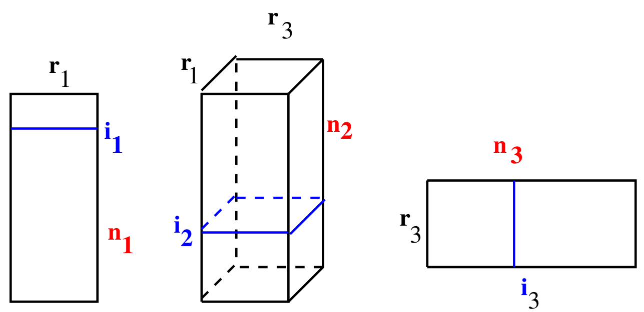
$$\mathbf{A} = \sum_{k=1}^{R} c_k \mathbf{u}_k^{(1)} \otimes \ldots \otimes \mathbf{u}_k^{(d)} = \mathbf{C} \times_1 U^{(1)} \times_2 U^{(2)} \ldots \times_d U^{(d)},$$



Reduced HOSVD (RHOSVD) of side matrices, <u>no need for full size tensor</u> :

$$U^{(\ell)} \approx Z_r^{(\ell)} \Sigma_r^{(\ell)} W_r^{(\ell)}, \quad U_r^{(\ell)} \in \mathbb{R}^{n_\ell \times r}, \quad r \ll R$$

Complexity of RHOSVD: $O(nR)$, no dependence on d!



[Khoromskij & Khoromskaia '09]

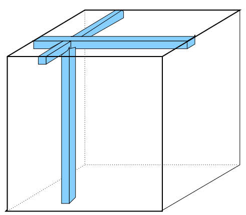
In grid-based calculation of the 3D convolution integrals with the Newton kernel in quantum chemistry there is a problem of rank reduction for tensors with
– large canonical ranks ($R \sim 10^4$) and
– on large $n \times n \times n$ 3D Cartesian grids, $n \sim 10^4 \div 10^5$.

$$\boldsymbol{\mathcal{C}}_{R,\mathbf{n}} \quad \overset{I}{\to} \quad \boldsymbol{\mathcal{T}}_{\mathbf{r},\mathbf{n}} \quad \overset{II}{\to} \quad \boldsymbol{\mathcal{T}}_{\mathcal{C}_{R'},\mathbf{r}} \quad \overset{III}{\to} \quad \boldsymbol{\mathcal{C}}_{R',\mathbf{n}}, \qquad R' \ll R.$$

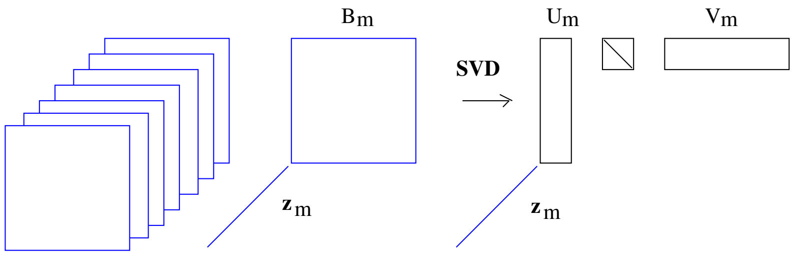
For full format tensors, the two-level F2T + T2C can be described as the following computation chain,

$$\mathbb{V}_{\mathbf{n}} \overset{I}{\to} \boldsymbol{\mathcal{T}}_{\mathbf{r},\mathbf{n}} \overset{II}{\to} \boldsymbol{\mathcal{T}}_{\mathcal{C}_{R},\mathbf{r}} \overset{III}{\to} \boldsymbol{\mathcal{C}}_{R,\mathbf{n}},$$

Tucker-to canonical transform (T2C) is based on canonical decomposition of the (small) core tensor with the rank bound: $R' \leq r^2$.



either



From history of sparse grid-based and tensor techniques

- Wavelets with canonical format, sparse grids. **[Harrison, Beylkin, Schwab, Schneider, Dahmen, Hackbusch, Griebel, Yserentant, Flad]**.
- Tensor-structured numerical methods: canonical-to-Tucker transform (RHOSVD), multigrid Tucker, 3D convolution integrals. **[Khoromskij, Khoromskaia (2006-2009)].**
- Tensor-based factorization of two-electron integrals, Hartree-Fock solvers. **[Khoromskaia, Khoromskij, Flad, Schneider (2009-2013)]**.
- Matrix Product States, Tensor Train (TT). **[White (1992), Oseledets, Tyrtyshnikov (2009)]**.
- Hierarchical Tucker (HT), hierar. SVD. **[Hackbusch, Kuhn, Grasedyck (2009)].**
- QTT format: quantics vector/tensor low rank approximation. **[Khoromskij (2009), Oseledets]**.
- Tensor methods for stochastic PDEs. **[Khoromskij, Schwab; Kressner, Tobler (2010)]**.
- TT-QTT format for solving chem. master equation, Fokker-Planck equation, HF. **[Khoromskij, Dolgov, Schwab, Kazeev, Oseledets, Rakhuba]**.
- Dynamical approximation by low-rank matrices and TT tensors. **[Lubich, Khoromskij, Oseledets, Schneider, Vandereycken]**.
- Collective electrostatics on 3D lattices with defects (2014). **[Khoromskaia, Khoromskij]**.
- Range-separated (RS) tensor format (2016), biomolecular modelling. **[Benner, Khoromskaia, Khoromskij]**.

Canonical tensor approx. of the Newton kernel

[Stenger '93] , [Hackbusch, Khoromskij '03-'06],

The Laplace-Gauss transform of the analytic radial basis (RB) functions $p(z) = p(\|x\|)$, $x \in \mathbb{R}^d$

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

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

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

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

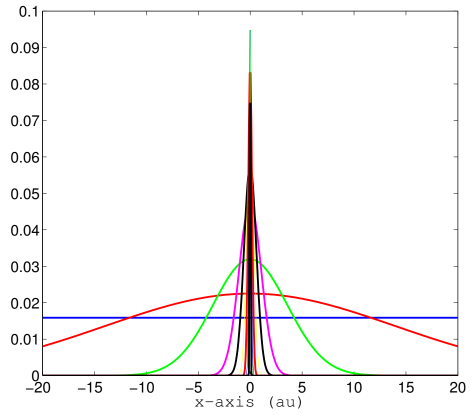
$$t_k = k\mathfrak{h}_M, \quad a_k = a(t_k)\mathfrak{h}_M, \quad \mathfrak{h}_M = C_0 \log(M)/M, \quad C_0 > 0.$$

$$\mathbf{P} \approx \mathbf{P}_R = \sum_{q=1}^{R} \mathbf{p}_q^{(1)} \otimes \mathbf{p}_q^{(2)} \otimes \mathbf{p}_q^{(3)} \in \mathbb{R}^{n \times n \times n}, \quad \mathbf{p}_q^{(\ell)} \in \mathbb{R}^{n_\ell}, \quad R \leq 2M+1 \approx C|\log \varepsilon|.$$

Numerical scheme for CP approx. of the Newton kernel

[Bertoglio, Khoromskij '08]

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



CPU times (Matlab) to generate $\mathbf{P}_N$, tolerance $\varepsilon = 10^{-6}$.

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

Was applied in 3D grid-based Hartree-Fock calculations (on $n \times n \times n$ grids with $n = 10^5$) **[Khoromskaia, Khoromskij 2008-2014]**.

Direct tensor summation

[Khoromskaia & Andrae & Khoromskij, CPC '12]

Nuclear potential operator: $V_c(x) = -\sum_{a=1}^{A} \frac{Z_a}{\|x - x_a\|}, \quad Z_a > 0, \;\; x, \; x_a \in \mathbb{R}^3$

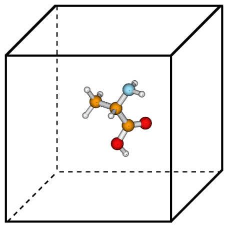
Reference tensor

$$\widehat{\mathbf{P}}_R = \sum_{q=1}^{R_N} \widehat{\mathbf{p}}_q^{(1)} \otimes \widehat{\mathbf{p}}_q^{(2)} \otimes \widehat{\mathbf{p}}_q^{(3)} \in \mathbb{R}^{2n \times 2n \times 2n},$$

and shifting/windowing operator $\mathcal{W}_a = \mathcal{W}_a^{(1)} \otimes \mathcal{W}_a^{(2)} \otimes \mathcal{W}_a^{(3)}$.

$$V_c \approx \mathbf{P}_c = \sum_{a=1}^{A} Z_a \mathcal{W}_a \widehat{\mathbf{P}}_R = \sum_{a=1}^{A} Z_a \sum_{q=1}^{R} \mathcal{W}_a^{(1)} \widehat{\mathbf{p}}_q^{(1)} \otimes \mathcal{W}_a^{(2)} \widehat{\mathbf{p}}_q^{(2)} \otimes \mathcal{W}_a^{(3)} \widehat{\mathbf{p}}_q^{(3)} \in \mathbb{R}^{n \times n \times n},$$

Rank of $\mathbf{P}_c$ is $R_N A$, where A is the number of nuclei in a molecule.



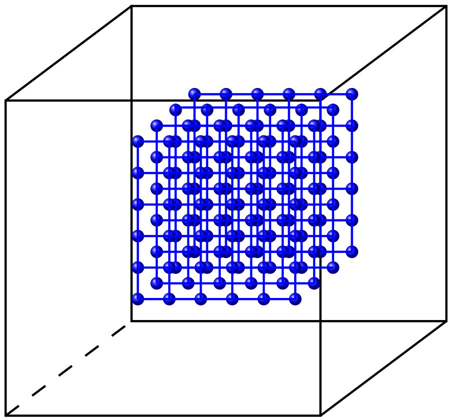
Large crystalline-type systems

Computation of the (free space) collective electrostatic potential of charged particles on large $L \times L \times L$ finite lattices (Newton kernels).
The electrostatic potential

$$V_c(x) = \sum_{i=1}^{L^3} \frac{Z_i}{\|x - x_i\|}, \; x \in \mathbb{R}^3,$$

and interaction energy of charged particles,

$$E_{nuc} = \sum_{i=1}^{L^3} \sum_{j<i}^{L^3} \frac{Z_i Z_j}{\|x_i - x_j\|}.$$



Classical methods for long-range potential sums

Classical methods in 3D many-particle modelling: Ewald summation and fast multipole method **[Ewald, 1927], [Greengard, Rochlin '87]**

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

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

Tensor summation by assembled canonical/Tucker vectors

[Khoromskaia & Khoromskij '14]

Theorem

Given rank-R reference canonical tensor $\mathbf{P}_N$, the collective electrostatic potential $v_{c_L}(x)$, $x \in \Omega_L$, of L^3 charges on a rectangular lattice $L \times L \times L$, is presented by the canonical tensor $\mathbf{P}_{c_L}$ of the same rank R,

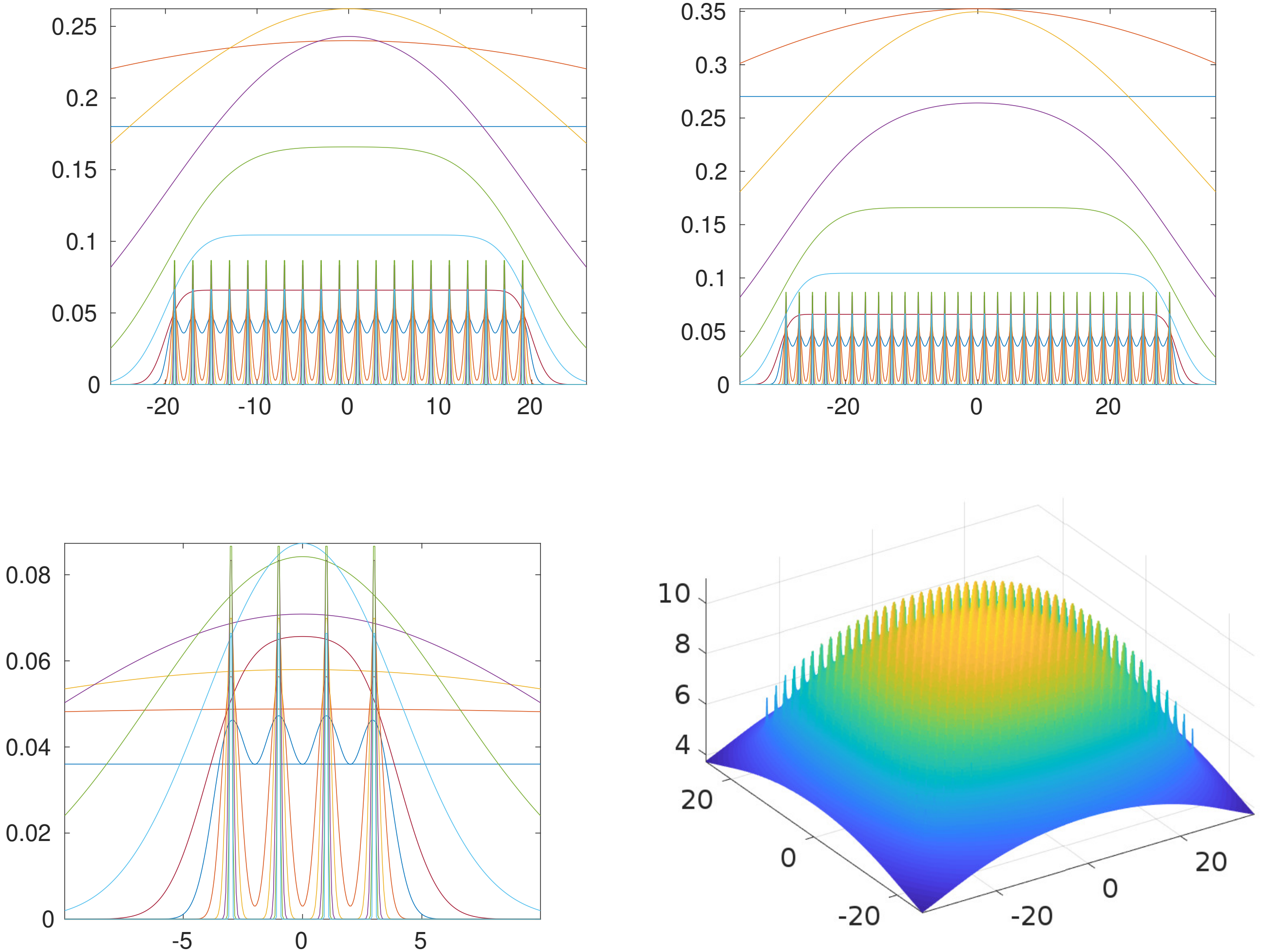
$$\mathbf{P}_{c_L} = \sum_{q=1}^{R} \Big(\sum_{k_1=1}^{L} \mathcal{W}_{(k_1)} \mathbf{p}_q^{(1)} \Big) \otimes \Big(\sum_{k_2=1}^{L} \mathcal{W}_{(k_2)} \mathbf{p}_q^{(2)} \Big) \otimes \Big(\sum_{k_3=1}^{L} \mathcal{W}_{(k_3)} \mathbf{p}_q^{(3)} \Big), \qquad (1)$$

where the 3D shift vector is defined by $\mathbf{k} \in \mathbb{Z}^{L \times L \times L}$, $\mathcal{W}_{(\mathbf{k})} = \mathcal{W}_{(k_1)}^{(1)} \otimes \mathcal{W}_{(k_2)}^{(2)} \otimes \mathcal{W}_{(k_3)}^{(3)}$. The numerical cost and storage are $O(RLn_L)$ and $O(Rn_L)$.

$\Rightarrow$ The rank of the collective electrostatic potential of charged particles on a large 3D finite lattice equals to a rank of a single Newton kernel.

Assembled canonical/Tucker vectors

Assembled vectors of the collective electrostatic potential for a cluster of $20 \times 30 \times 4$ Hydrogen atoms, 3D box $55.4 \times 33.6 \times 22.4$ au^3, (abs. accuracy 10^{-14}).



Superfast summation by tensor methods

Times (s) for calculation of the free-space collective electrostatic potential of charged particles on a 3D rectangular lattice (MATLAB, laptop)

L^3	64^3	128^3	256^3	512^3
charged particles	262144	2097152	$16 \cdot 10^6$	$134 \cdot 10^6$
n^3	4480^3	8576^3	16768^3	33152^3
time (s)	1.2	2.4	8.9	37.2
n^3	8960^3	17152^3	33536^3	66304^3 (10^{14})
time (s)	1.0	4.1	18.8	84.6

The caze of different charges: introduce the three-fold charge tensor $\mathbf{Z} = \{z_{k_1,k_2,k_3}\}$, $k_\ell = 1, \ldots, L$. Assume that tensor $\mathbf{Z}$ admits the rank-R_Z canonical decomposition

$$\mathbf{Z} = \sum_{m=1}^{R_Z} \mathbf{z}_m^{(1)} \otimes \mathbf{z}_m^{(2)} \otimes \mathbf{z}_m^{(3)}.$$

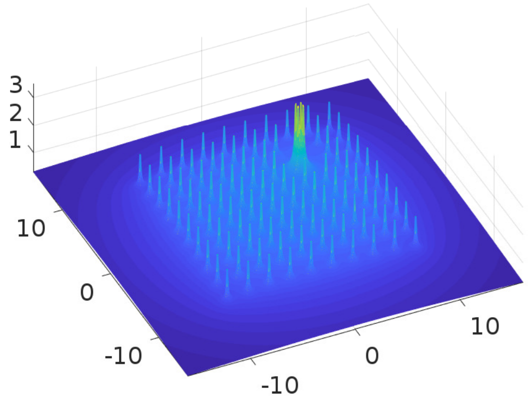
$$\mathbf{P}_{c_L} = \sum_{m=1}^{R_Z} \sum_{q=1}^{R} \Big(\sum_{k_1=1}^{L} z_{k_1,m}^{(1)} \mathcal{W}_{(k_1)} \mathbf{p}_q^{(1)} \Big) \otimes \Big(\sum_{k_2=1}^{L} z_{k_2,m}^{(2)} \mathcal{W}_{(k_2)} \mathbf{p}_q^{(2)} \Big) \otimes \Big(\sum_{k_d=1}^{L} z_{k_3,m}^{(3)} \mathcal{W}_{(k_3)} \mathbf{p}_q^{(3)}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

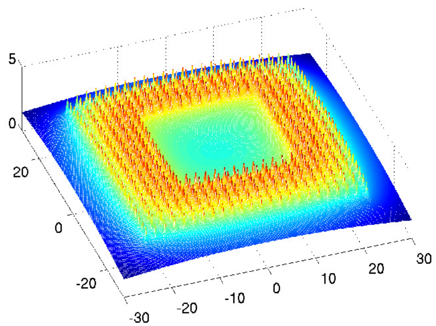
The numerical cost is $O(R_Z R L n)$. Rank of $\mathbf{P}_{c_L} \leq R_Z R$.

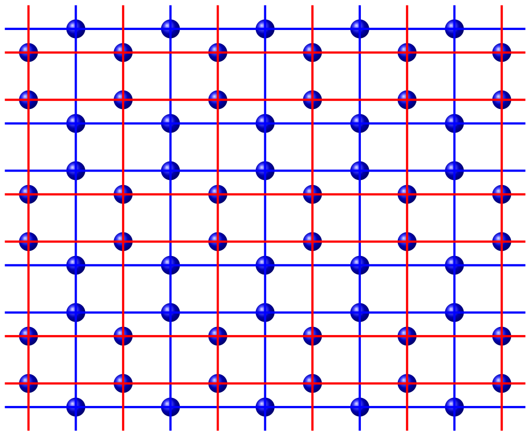
Tensor sums on composite geometries

[Khoromskaia & Khoromskij '14] The target lattice $\mathcal{L}$ is the union of several sub-lattices $\mathcal{L}_q$ represented on a 3D rectangular grid.

$$\mathcal{L} = \bigcup \mathcal{L}_q.$$







A hexagonal lattice is a union of two rectangular lattices, "red" and "blue".

Interaction energy of electrostatic potentials on a lattice

[Khoromskaia & Khoromskij '15]

$$E_{nuc} = \frac{1}{2} \sum_{i \neq j}^{L^3} \sum_{j=1}^{L^3} \frac{Z_i Z_j}{\|x_i - x_j\|}.$$

Having tensor $\mathbf{P}_{c_L}$, the energy sum with accuracy $O(h^2)$ is computed as

$$E_{nuc} \approx \frac{Z^2 h^{-3}}{2} (\langle \mathbf{p}_{c_L}, \mathbf{1} \rangle - \langle \mathbf{p}_{0L}, \mathbf{1} \rangle),$$

where $\mathbf{p}_{c_L}$ is a vector of samples of $\mathbf{P}_{c_L}$ at points x_i. Complexity $O(L^2) \ll L^3 \log L$.

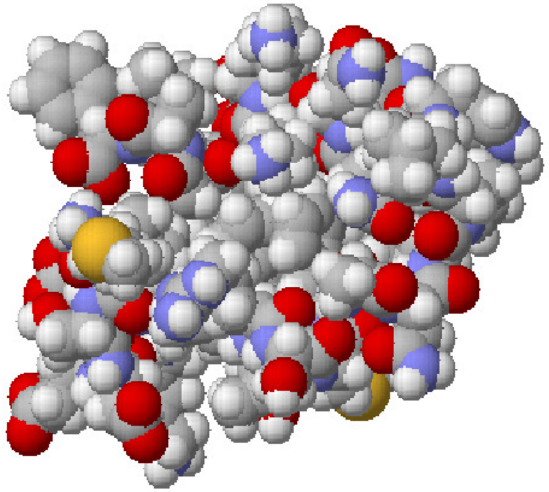
L^3	T_{full} $(O(L^3))$ (s)	$\mathrm{T}_{tens.}$ (s)	$E_{L,T}$	abs. err.
32^3	250, (15.8)	1.5	$1.5 \cdot 10^7$	$1.5 \cdot 10^{-9}$
48^3	3374, (58.8)	2.8	$1.12 \cdot 10^8$	0
64^3	–	5.7	$5.0 \cdot 10^8$	–
128^3	–	13.5	$1.6 \cdot 10^{10}$	–
$256^3 = 16 \cdot 10^6$	–	68.2	$5.2 \cdot 10^{11}$	–

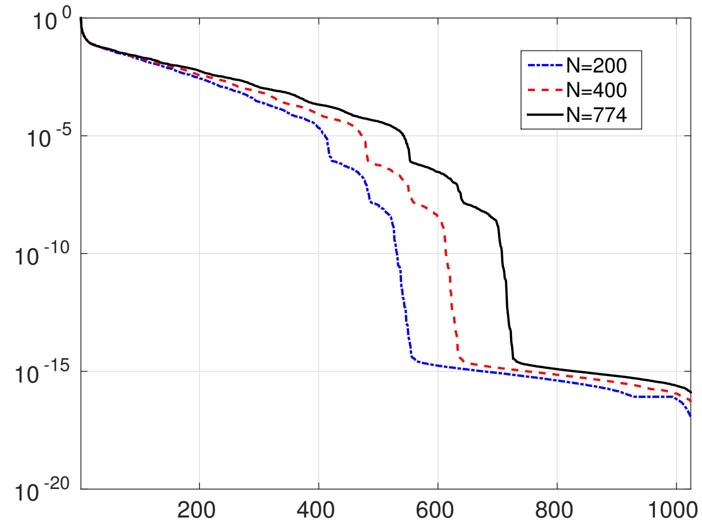
T_{full} indicates straightforward calculation of $O(L^6)$, brackets correspond to $O(L^3)$. $\mathrm{T}_{tens.}$ shows times for assembled tensor calculations.

Tensor summation of potentials for many-particle systems

What if a many-particle system is not on a lattice, like a protein?

Summation of canonical tensors yields large ranks ($R \sim N_0$) when the number of particles increases (a "disordered system")





Mode-1 singular values of the side matrix in the full potential sum vs. the number of particles $N_0 = 200, 400, 774$, $n = 1024$.

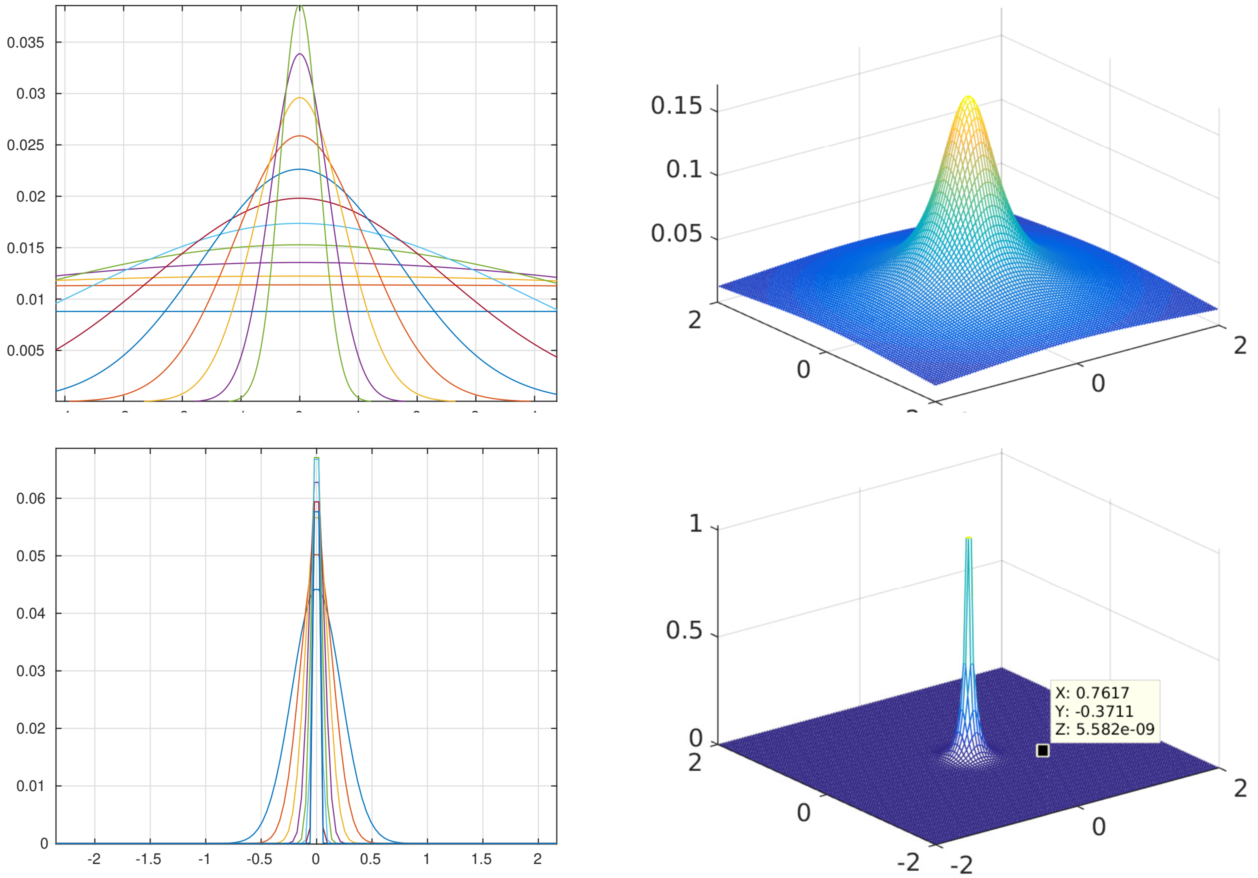
$$P_0(x) \mapsto \mathbf{P}_0 = \sum_{\nu=1}^{N_0} z_\nu \, \mathcal{W}_\nu(\widehat{\mathbf{P}}_R).$$

Range separation of a tensor for a single Newton kernel

[Benner & Khoromskaia & Khoromskij, SISC'18]

Preparatory step: range-separated representation of the CP tensor $\mathbf{P}_R$ (k is a partitioning parameter)

$$\mathbf{P}_R = \mathbf{P}_{R_s} + \mathbf{P}_{R_l} : \quad \mathbf{P}_{R_s} = \sum_{k \in \mathcal{T}_s} \mathbf{p}_k^{(1)} \otimes \mathbf{p}_k^{(2)} \otimes \mathbf{p}_k^{(3)}, \quad \mathbf{P}_{R_l} = \sum_{k \in \mathcal{T}_l} \mathbf{p}_k^{(1)} \otimes \mathbf{p}_k^{(2)} \otimes \mathbf{p}_k^{(3)}.$$

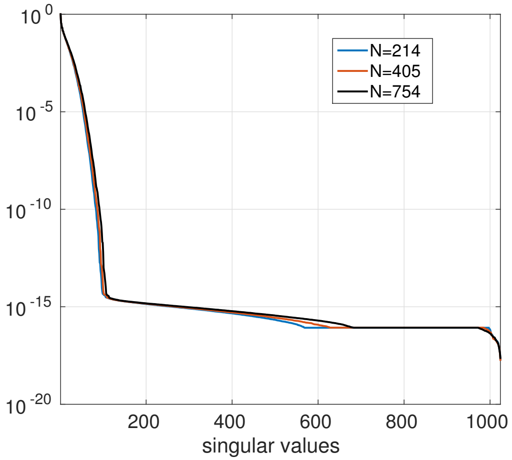


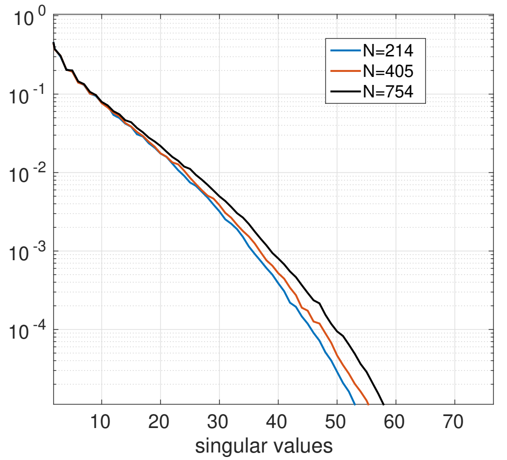
Remedy: new range-separated tensor format

[Benner & Khoromskaia & Khoromskij, SISC '18]

$$P_0(x) \mapsto \mathbf{P}_0 = \sum_{\nu=1}^{N_0} z_\nu \, \mathcal{W}_\nu(\widehat{\mathbf{P}}_R) = \sum_{\nu=1}^{N_0} z_\nu \, \mathcal{W}_\nu(\widehat{\mathbf{P}}_{R_s} + \widehat{\mathbf{P}}_{R_l}) := \mathbf{P}_s + \mathbf{P}_l.$$

Initial rank of the tensor $\mathbf{P}_l$ is huge: $N_0 R_l$ (exceeds 10^4). Not tractable!





Decay of singular values of side matrices for the long-range part $\mathbf{P}_l$ vs. N_0, $R_l = 12$, (nearly independent on the number of particles).

We apply the RHOSVD and C2T + T2C algorithms to reduce the canonical rank of tensor $\mathbf{P}_l$ up to $200 \div 400$.

Rank bounds for long-range part

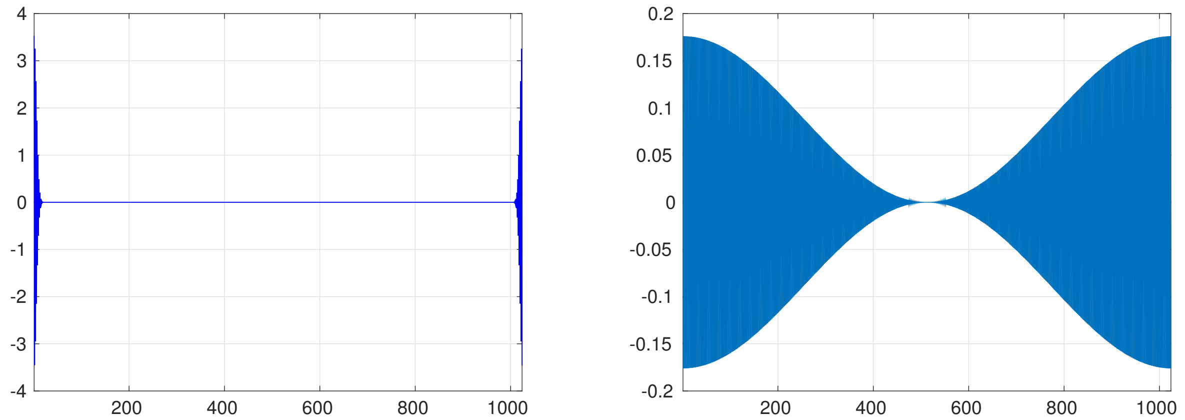
[Benner & Khoromskaia & Khoromskij, SISC '18]

Theorem

Let the long-range part $\mathbf{P}_l$ in the total interaction potential, correspond to the choice of splitting parameter $M/2$ with $M = O(\log^2 \varepsilon)$. Then the total ε-rank $\mathbf{r}_0$ of the Tucker approximation to the canonical tensor sum $\mathbf{P}_l$ is bounded by

$$|\mathbf{r}_0| := rank_{Tuck}(\mathbf{P}_l) = C\, b \log^{3/2}(\log 1/\varepsilon + \log N),$$

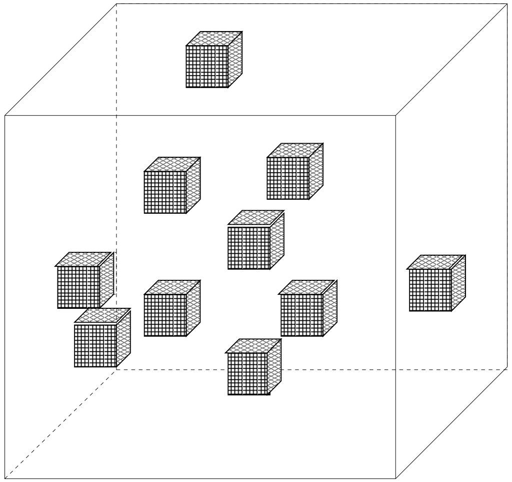
where the constant C does not depend on the number of particles N.

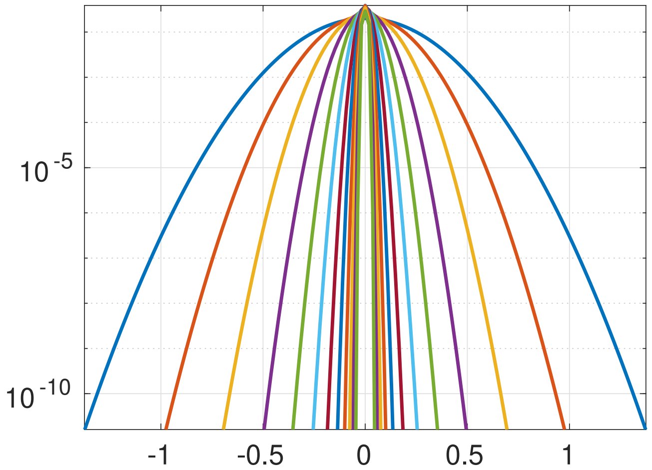


Fourier coefficients of the long- (left) and short-range (right) discrete Gaussians.

Range-separated tensor format

What about the short-range part of potentials?





Definition

(Cumulated canonical tensors, CCT). A rank-R_0 CCT, $\mathbf{U}$, associated with $\mathcal{J}$ and separation parameter γ, is defined as a set of tensors which can be represented by

$$\mathbf{U} = \sum\nolimits_{\nu=1}^{N_0} c_\nu \mathbf{U}_\nu, \quad \text{with} \quad rank(\mathbf{U}_\nu) \leq R_0, \tag{2}$$

where the can. tensors $\mathbf{U}_\nu = [u_{\mathbf{j}}]$ are vanishing beyond the γ-vicinity of $\mathbf{j}^{(\nu)}$.

Range-separated tensor format

[Benner & Khoromskaia & Khoromskij SISC'18]

Definition

(RS-canonical tensors). The RS-canonical tensor format defines the class of d-tensors $\mathbf{A} \in \mathbb{R}^{n_1 \times \cdots \times n_d}$, which can be represented as a sum of a (low) rank-R canonical tensor $\mathbf{U}$ and a (uniform) cumulated canonical tensor generated by $\mathbf{U}_0$ with $\operatorname{rank}(\mathbf{U}_0) \leq R_0$,

$$\mathbf{A} = \sum\nolimits_{k=1}^{R} \xi_k \mathbf{u}_k^{(1)} \otimes \cdots \otimes \mathbf{u}_k^{(d)} + \sum\nolimits_{\nu=1}^{N_0} c_\nu \mathbf{U}_\nu, \quad \text{where} \quad \operatorname{diam}(\operatorname{supp} \mathbf{U}_\nu) \leq 2\gamma. \tag{3}$$

Lemma

The storage cost of RS-canonical tensor is estimated by

$$stor(\mathbf{A}) \leq dRn + (d+1)N_0 + dR_0\gamma.$$

RS tensors differ from the conventional tensor formats due to their intrinsic features, originating from tensor approximation to multivariate functions with multiple singularities.

RS repr. of the free-space electrost. potential in a protein

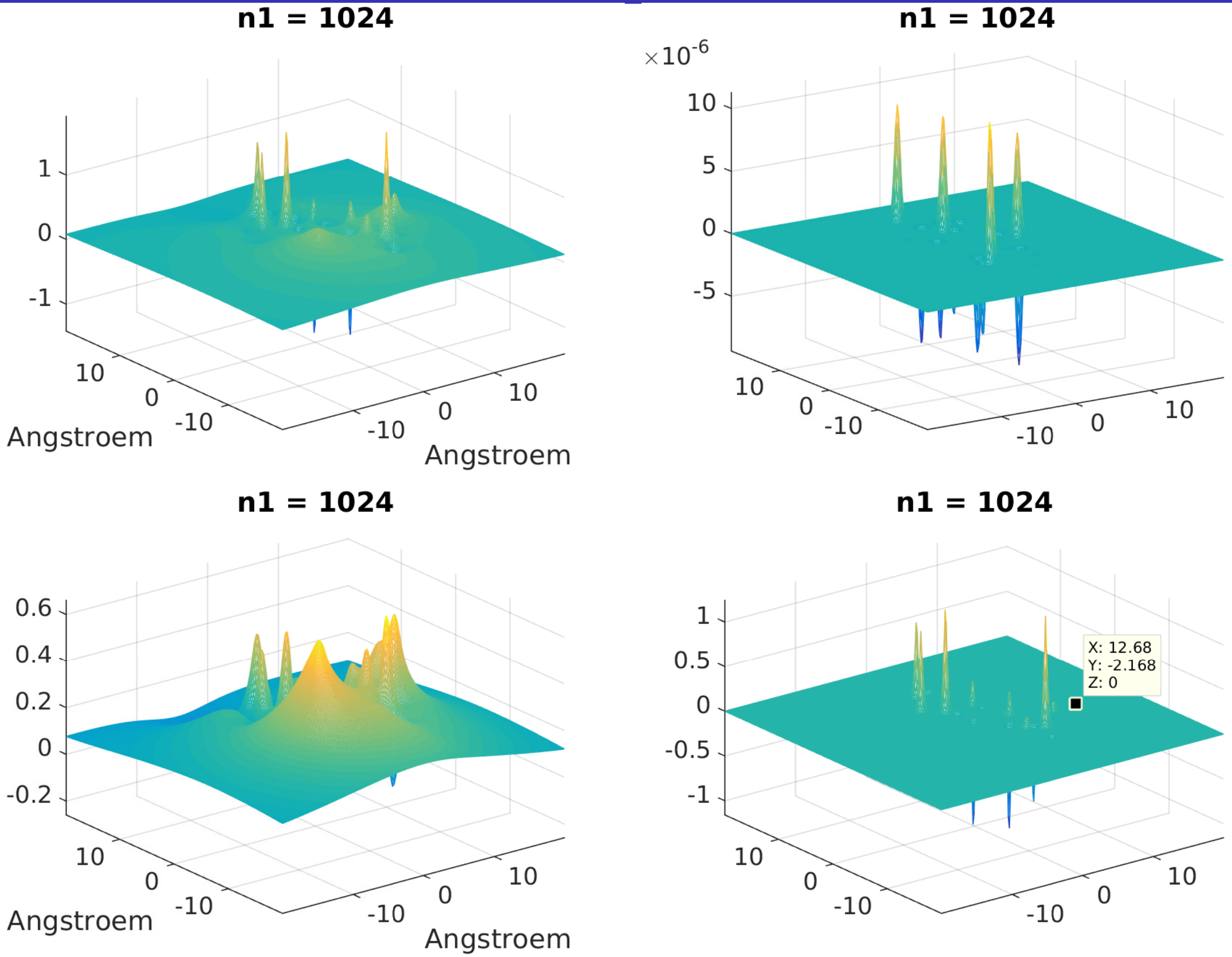


Figure: *Top: the potential sum at a middle plane of a cluster with* **400 atoms** *(left), and the error of the RS-canonical approximation (right). Bottom: long-range part of a sum (left), short range part of a sum (right).*

Interaction energy

Lemma

The interaction energy E_N of the N-particle system can be calculated by using only the long range part in the total potential sum

$$E_N = E_N(x_1, \dots, x_N) = \frac{1}{2} \sum_{j=1}^{N} z_j (\mathbf{P}_l(x_j) - z_j \mathbf{P}_{R_l}(x = 0)), \tag{4}$$

in $O(dR_l N)$ operations, where R_l is the canonical rank of the long-range component.

Further research in biomolecular modeling:

- B. N. Khoromskij. Range-separated tensor decomposition of the discretized Dirac delta and elliptic operator inverse. J Comp. Phys. 401, 108998, 2020.
- P. Benner, V. Khoromskaia, B. N. Khoromskij, C. Kweyu, M. Stein. Regularization of Poisson–Boltzmann Type Equations with Singular Source Terms Using the Range-Separated Tensor Format. SIAM J Sci. Comput. 43 (1), A415-A445, 2021.

Prospects:

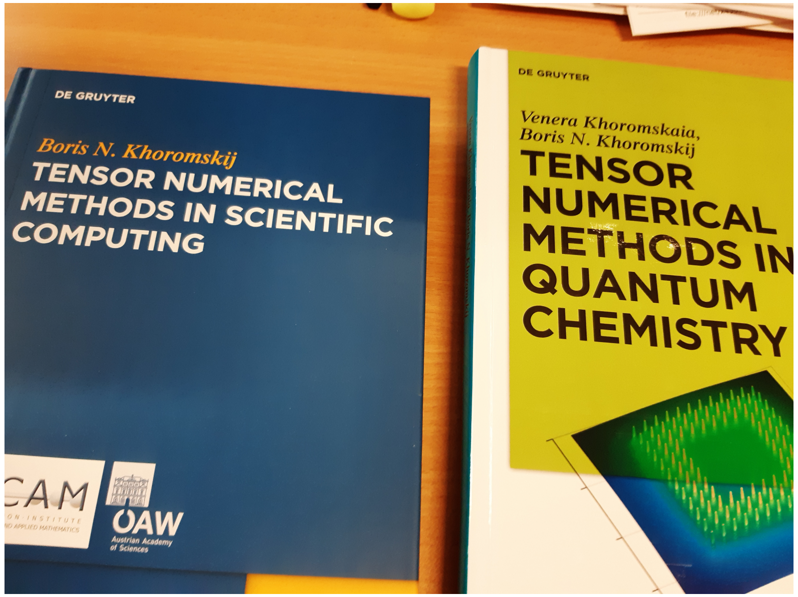
- **Collective (free space) electrostatic potential of nanostructures and small crystalline-type systems.**
- **Application of the RS tensor format for protein docking problem.**

Tensor-based methods, what is next?

Some other results and perspectives of the tensor-structured approaches:

- Grid-based numerical solution of the 3D Hartree-Fock equation, **[Khoromskaia, Khoromskij, Flad, Schneider '09-'15]**. Excitation energies and optical spectra of molecules **[Benner, Khoromskaia, Khoromskij, Dolgov, Yang, '16-'19]**.
- Analysis of QTT approximation for classes of functions and operators **[Khoromskij, Oseledets, Dolgov, Kazeev, Rakhuba, Hackbusch, Schwab, '09-'20]**
- Tensor-based methods for stochastic PDEs **[Khoromskij, Schwab, Oseledets]**,
- Tensor-based 3D preconditioners for elliptic partial differential equations in 3D, for stohastic homogenization problem **[Khoromskaia, Khoromskij, Otto '2020]**.
- Geometry of tensor manifolds, tensors in nonlinear algebra and algebraic geometry **[Sturmfels, Seigal, Michalek, Pfeffer, Robeva, Telen, '16-'21]**.
- Nonlinear approximation theory for tensors in data science **[Uschmajew, Bachmayr, Hackbusch, Schneider, Chichoki, Oseledets, Vandereycken]**.
- Tensor method for optimal control problems with fractional multidimensional Laplacian in constraints **[Khoromskij, Schulz, Khoromskaia, Heidel, Schmitt '18-'20]**.

Tensor numerical methods and their applications



Boris N. Khoromskij.
Tensor Numerical Methods in Scientific Computing
De Gruyter, Berlin, 2018.

Venera Khoromskaia, Boris N. Khoromskij.
Tensor Numerical Methods in Quantum Chemistry
De Gruyter, Berlin, 2018.

Thank you for your attention !