15 Lectures on Tensor Numerical Methods for Multi-dimensional PDEs

Lect. 15. Superfast tensor summation of of electrostatic potentials on 3D lattices.

New range-separated tensor format for multiparticle systems.

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Outline of the lecture

1. Tensor-based summation of long-range potentials on 3D lattices
   - Grid-based canonical representation of the Newton kernel
   - Direct tensor summation of 3D potentials in 1D complexity
   - Lattice sums by tensor approach : $O(L)$ instead of $O(L^3)$
   - Tensor sums on composite geometries
   - Interaction energy of elect. potentials on 3D lattices

2. Tensor summation of potentials for 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

[Stenger '89], [Braess '95], [Gavrilyuk, Hackbusch, Khoromskij '05], [Bertoglio, Khoromskij '08]

$$\mathbf{P} := [p_{\mathbf{i}}] \in \mathbb{R}^{n\times n\times n}, \quad p_{\mathbf{i}} = \int_{\mathbb{R}^3} \frac{\psi_{\mathbf{i}}(\mathbf{x})}{\|\mathbf{x}\|} d\mathbf{x}, \quad \psi_{\mathbf{i}}(\mathbf{x}) = \prod_{\ell=1}^{d} \psi_{i_\ell}^{(\ell)}(x_\ell), \ \{i_\ell\}_1^{n_\ell}, \ \ell = 1, 2, 3.$$

Start with the Laplace-Gauss transform for the analytic function p(z), with a weight $a(t) > 0$,

$$p(z) = \int_{\mathbb{R}_+} a(t) e^{-t^2 z^2} \, dt \approx \sum_{k=-M}^{M} a_k e^{-t_k^2 z^2} \quad \text{for} \quad |z| > 0,$$

where the quadrature points and weights are given by

$$t_k = k\hbar_M, \quad a_k = a(t_k)\hbar_M, \quad \hbar_M = C_0 \log(M)/M, \quad C_0 > 0.$$

For a particular case $p(z) = 1/z$, $z = \sqrt{x_1^2 + x_2^2 + x_3^2}$, we apply the Laplace-Gauss transform

$$\frac{1}{z} = \frac{2}{\sqrt{\pi}} \int_{\mathbb{R}_+} e^{-t^2 z^2} dt, \quad \text{i.e.} \quad a(t) = \frac{2}{\sqrt{\pi}}.$$

A canonical tensor for Newton kernel $\frac{1}{\|\mathbf{x}\|}$

Now for any fixed $x = (x_1, x_2, x_3) \in \mathbb{R}^3$, such that $\|x\| > 0$, we apply the sinc-quadrature approximation to obtain the separable expansion

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

Under the assumption $0 < a \le \|x\| \le A < \infty$ sinc-approximation provides the exponential convergence rate in M,

$$\left| p(\|x\|) - \sum_{k=-M}^{M} a_k e^{-t_k^2\|x\|^2} \right| \le \frac{C}{a} e^{-\beta\sqrt{M}}, \quad \text{with some } C, \beta > 0.$$

A canonical tensor for Newton kernel $p(\|x\|) = \frac{1}{\|\mathbf{x}\|}$

[Bertoglio, Khoromskij '08]
Combining above relations and taking into account the separability of the Gaussian basis functions, we arrive at the low-rank approximation to each entry of the tensor $\mathbf{P}$,

$$p_{\mathbf{i}} \approx \sum_{k=-M}^{M} a_k \int_{\mathbb{R}^3} \psi_{\mathbf{i}}(\mathbf{x}) e^{-t_k^2 \|x\|^2} \mathrm{d}x = \sum_{k=-M}^{M} a_k \prod_{\ell=1}^{3} \int_{\mathbb{R}} \psi_{i_\ell}^{(\ell)}(x_\ell) e^{-t_k^2 x_\ell^2} \mathrm{d}x_\ell.$$

Define the vector (recall that $a_k > 0$) $\mathbf{p}_k^{(\ell)} = a_k^{1/3} \mathbf{b}^{(\ell)}(t_k) \in \mathbb{R}^{n_\ell}$, where

$$\mathbf{b}^{(\ell)}(t_k) = \left[b_{i_\ell}^{(\ell)}(t_k) \right]_{i_\ell=1}^{n_\ell} \in \mathbb{R}^{n_\ell} \quad \text{with} \quad b_{i_\ell}^{(\ell)}(t_k) = \int_{\mathbb{R}} \psi_{i_\ell}^{(\ell)}(x_\ell) e^{-t_k^2 x_\ell^2} \mathrm{d}x_\ell.$$

The 3rd order tensor $\mathbf{P}$ can be approximated by the R-term canonical representation

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

where $R = 2M + 1$.

Tensor-based nuclear potential operator (for molecules)

[Khoromskaia, Andrae, Khoromskij, CPC '12],

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

Reference tensor

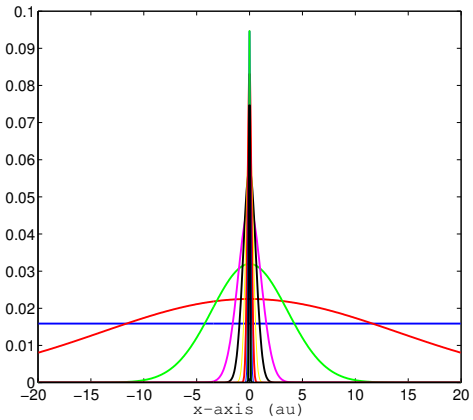
$$\widetilde{\mathbf{P}}_R = \sum_{q=1}^{R} \widetilde{\mathbf{p}}_q^{(1)} \otimes \widetilde{\mathbf{p}}_q^{(2)} \otimes \widetilde{\mathbf{p}}_q^{(3)} \in \mathbb{R}^{2n \times 2n \times 2n},$$

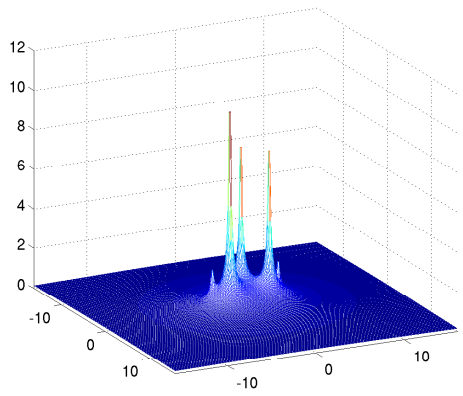
and shifting/windowing operator $\mathcal{W}_a = \mathcal{W}_a^{(1)} \otimes \mathcal{W}_a^{(2)} \otimes \mathcal{W}_a^{(3)}$.
Direct tensor summation: $O(A)$, where A is the number of atoms in a molecule.

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

$$\overline{v}_{\mu\nu} = \int_{\mathbb{R}^3} V_c(x) \overline{g}_\mu(x) \overline{g}_\nu(x) dx \approx \langle \mathbf{G}_\mu \odot \mathbf{G}_\nu, \mathbf{P}_c \rangle, \quad 1 \le \mu, \nu \le N_b.$$

[Khoromskaia, CMAM '13]





Left: Examples of vectors of the canonical tensor representation of the Newton kernel (here x-axis).
Right: Computed V_c for ethanol molecule (C_2H_5OH),
$n^3 = 10^{15}$, mesh-size $h \sim 1.164 \cdot 10^{-4}$ Å $= 11.64$ fm.

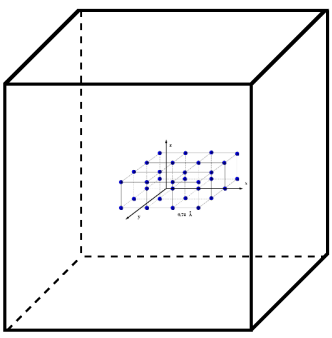
Large crystalline-type systems

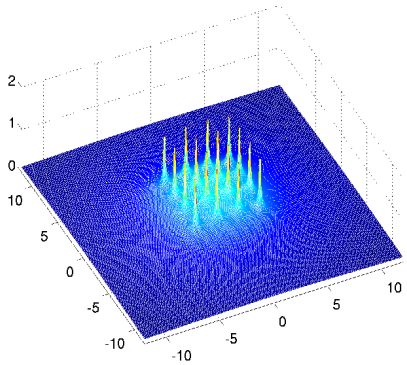
[Khoromskaia, Khoromskij CPC'14], **[Khoromskaia, Khoromskij NLAA'16]**

One of the main problems:

- Computing large $L \times L \times L$ lattice sums of long range electrostatic potentials (Newton kernels).

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





Classical methods for long-range potential sums

Summation of long-range potentials in a volume is a classical problem in 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,

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

$\Rightarrow O(L^3)$ instead of $O(L^6)$ for direct sum $E_{nuc} = \sum_{i=1}^{L^3} \sum_{j<i}^{L^3} \frac{Z_i Z_j}{r_{ij}}$, $r_{ij} = \|x_i - x_j\|$.

Tensor-based sums by canonical/Tucker tensors

[VK, Khoromskij '14]

Theorem

Given rank-R canonical tensor $\mathbf{P}_N$, the electrostatic potential $v_{c_L}(x)$, $x \in \Omega_L$, of the full lattice sum over L^3 charges can be presented by the canonical tensor $\mathbf{P}_{c_L}$ of the same rank R,

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

The numerical cost and storage size are estimated by $O(RLn_L)$ and $O(Rn_L)$, where n_L is the univariate grid size.

We consider the sum of potentials defined on the domain Ω_L,

$$v_{c_L}(x) = \sum_{k_1,k_2,k_3=1}^{L} \frac{Z}{\|x - b\mathbf{k}\|}, \quad x \in \Omega_L. \tag{3}$$

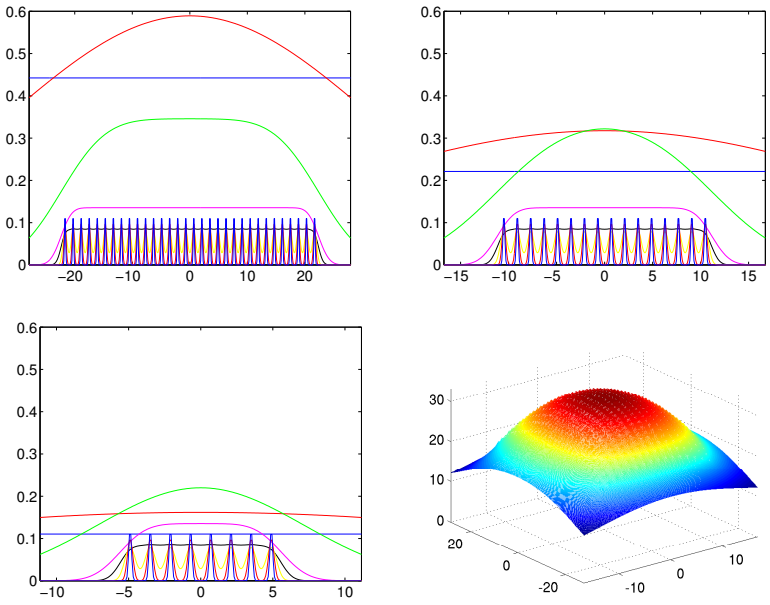
Then the projected tensor representation of $v_{c_L}(x)$ takes the form (omitting factor Z)

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

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

Tensor-based summation assembled canonical/Tucker vectors

[VK, Khoromskij '14] Assembled vectors of the tensor representing a sum of lattice electrostatic potentials (abs. accuracy 10^{-14}).



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

Superfast summation by tensor methods

Times for grid-based calculation of long-range potentials on a lattice (MATLAB, laptop)

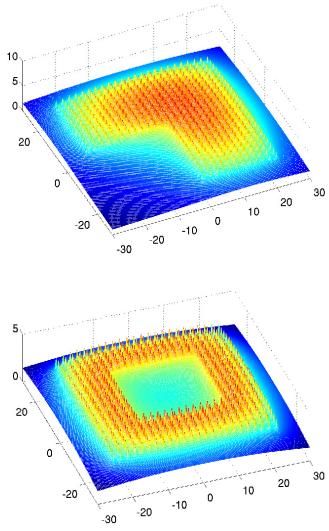
Size of 3D lattice L^3	64^3	128^3	256^3	512^3
number of particles	262144	2097152	$16 \cdot 10^6$	$134 \cdot 10^6$
size in nanometers^3	7^3	13.4^3	26.2^3	51.8^3
$h_0 = 3 \cdot 10^{-2}$ Å, grid size n^3	2240^3	4288^3	8384^3	16576
Time (s)	0.35	1.0	3.47	27.6
$h_0 = 1.5 \cdot 10^{-2}$ Å, grid size n^3	4480^3	8576^3	16768^3	33152^3
Time (s)	1.2	2.4	8.9	37.2
$h_0 = 8 \cdot 10^{-3}$ Å, grid size n^3	8960^3	17152^3	33536^3	66304^3 (10^{14})
Time (s)	1.0	4.1	18.8	84.6

Note that for every tensor summation the single reference Newton kernel is generated on the grid which is two times larger ($2n$) than the size of the total grid in a box.

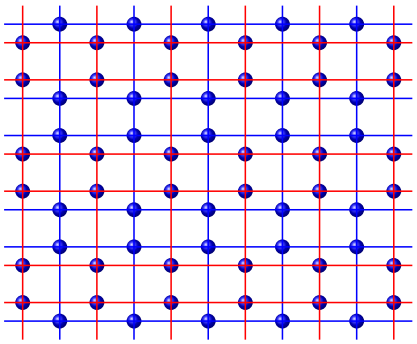
Tensor sums on composite geometries

[V. Khoromskaia, Khoromskij '14] The target lattice $\mathcal{L}$ can be split into the union of several sub-lattices, such that each sub-lattice $\mathcal{L}_q$ is represented on a 3D rectangular grid.

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

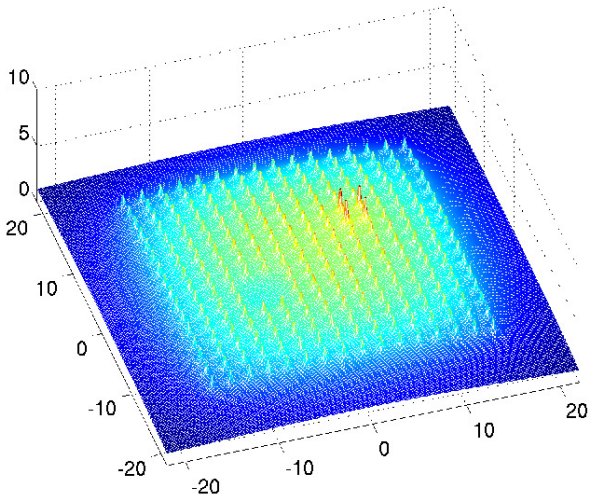


$A_{sum} = A_1 - A_2$



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

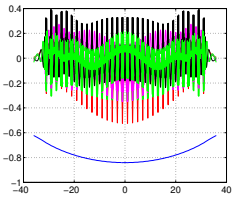
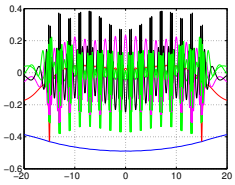
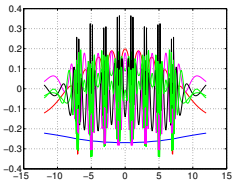
Tensor sums on composite geometries



Tucker tensor sums: rank-reduction for composite geometries

For multiple defects: Tucker tensor representation of the Newton kernel by the Canonical-to-Tucker algorithm

$$\mathbf{T}_{c_L} = \sum_{m_1=1}^{r_1}\sum_{m_2=1}^{r_2}\sum_{m_2=1}^{r_2} b_{m_1,m_2,m_3}\Big(\sum_{k_1=1}^{L}\mathcal{W}_{(k_1)}\widetilde{\mathbf{t}}^{(1)}_{m_1}\Big)\otimes\Big(\sum_{k_2=1}^{L}\mathcal{W}_{(k_2)}\widetilde{\mathbf{t}}^{(2)}_{m_2}\Big)\otimes\Big(\sum_{k_3=1}^{L}\mathcal{W}_{(k_3)}\widetilde{\mathbf{t}}^{(3)}_{m_3}\Big).$$

$$\mathbf{T}_{c_L} \mapsto \widehat{\mathbf{U}} = \mathbf{U}_0 + \sum_{s=1}^{S}\mathbf{U}_s$$

L^3	4096	32768	262144	2097152
Time (s)	1.8	0.8	3.1	15.8
N^3	5632^3	9728^3	17920^3	34304^3

Interaction energy of electrostatic potentials on a lattice

[Khoromskaia, Khoromskij '15]

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

$$E_{L,T} = \frac{Z^2 h^{-3}}{2}\big(\langle\widehat{\mathbf{P}}_{c_L},\mathbf{1}\rangle - \sum_{\mathbf{k}\in\mathcal{K}}\mathbf{P}_{|x_{\mathbf{k}}=0}\big),$$

By using the rank-1 tensor $\mathbf{P}_{0L} = \mathbf{P}_{|x_{\mathbf{k}}=0}\mathbf{1}$, the correction term can be represented by a simple tensor operation

$$\sum_{\mathbf{k}\in\mathcal{K}}\mathbf{P}_{|x_{\mathbf{k}}=0} = \langle\mathbf{P}_{0L},\mathbf{1}\rangle.$$

Finally, the interaction energy E_L allows the approximate representation

$$E_L \approx E_{L,T} = \frac{Z^2 h^{-3}}{2}\big(\langle\widehat{\mathbf{P}}_{c_L},\mathbf{1}\rangle - \langle\mathbf{P}_{0L},\mathbf{1}\rangle\big), \qquad (4)$$

that can be implemented in $O(L^2) \ll L^3 \log L$ complexity.

Interaction energy of electrostatic potentials on a lattice

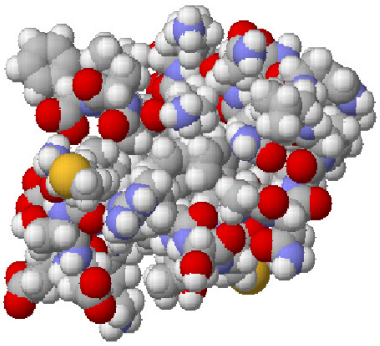
L^3	T_{full} (s), $(O(L^3))$	$T_{tens.}$ (s)	$E_{L,T}$	abs. err.
24^3	37, (6.1)	1.2	$3.7 \cdot 10^6$	$2 \cdot 10^{-8}$
32^3	250, (15.8)	1.5	$1.5 \cdot 10^7$	$1.5 \cdot 10^{-9}$
48^3	3374, (58.8)	2.8	$1.12 \cdot 10^8$	0
64^3	–	5.7	$5.0 \cdot 10^8$	–
128^3	–	13.5	$1.6 \cdot 10^{10}$	–
256^3	–	68.2	$5.2 \cdot 10^{11}$	–

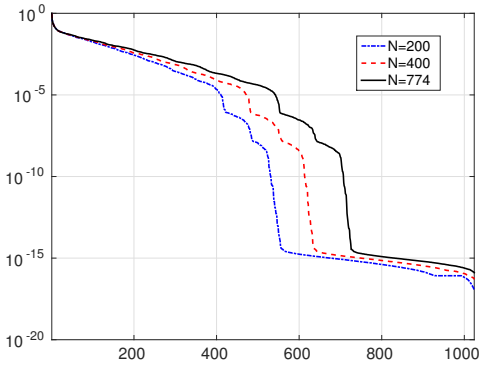
Times for computation of the interaction energy of electrostatic potentials on large finite lattices (in seconds).
T_{full} indicates straightforward calculation of $O(L^6)$, numbers in brackets are corresponding square roots.
$T_{tens.}$ shows times for assembled tensor calculations.

Tensor summation of potentials for many-particle systems

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

Summation of canonical tensors yields large ranks when the number of particles increases ("disordered system")





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

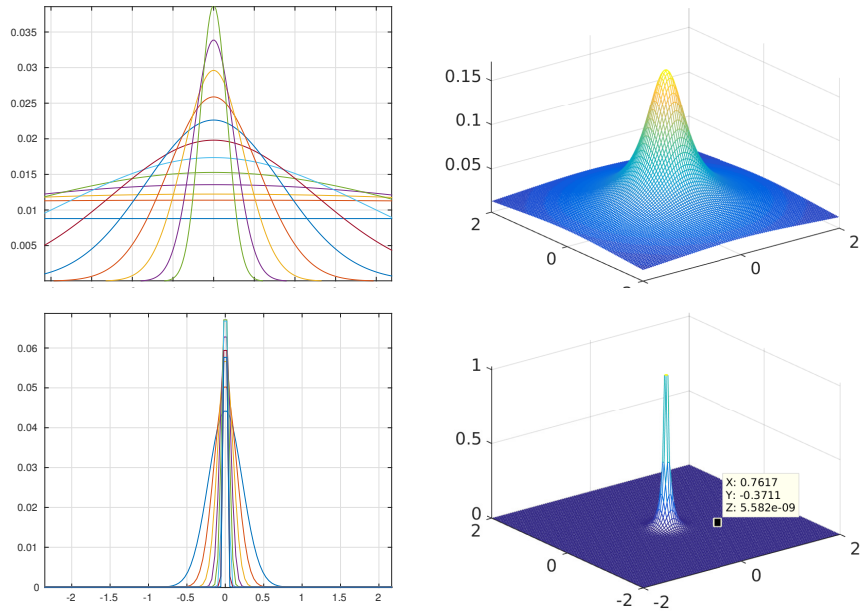
$$P_0(x) \mapsto \mathbf{P}_0 = \sum_{\nu=1}^{N_0} z_\nu \, \mathcal{W}_\nu(\widetilde{\mathbf{P}}_R).$$

Range separation of a tensor for a single Newton kernel

[Benner, Khoromskaia, Khoromskij, arXiv '16]

Preparatory step 1: Additive range-separated decomposition of the CP tensor $\mathbf{P}_R$

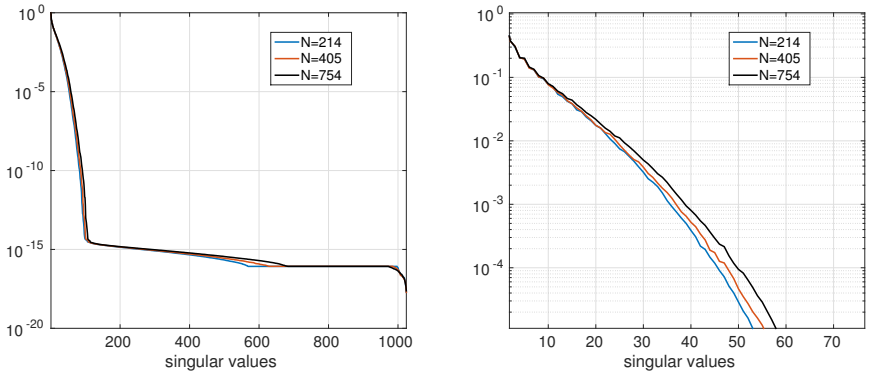
$$\mathbf{P}_R = \mathbf{P}_{R_s} + \mathbf{P}_{R_l}: \quad \mathbf{P}_{R_s} = \sum_{k\in\mathcal{T}_s} \mathbf{p}_k^{(1)} \otimes \mathbf{p}_k^{(2)} \otimes \mathbf{p}_k^{(3)}, \quad \mathbf{P}_{R_l} = \sum_{k\in\mathcal{T}_l} \mathbf{p}_k^{(1)} \otimes \mathbf{p}_k^{(2)} \otimes \mathbf{p}_k^{(3)}.$$



Remedy: new range-separated tensor format

[Benner, Khoromskaia, Khoromskij, arXiv '16]

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

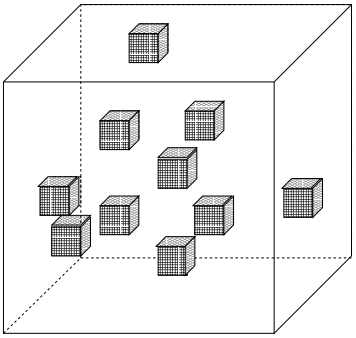


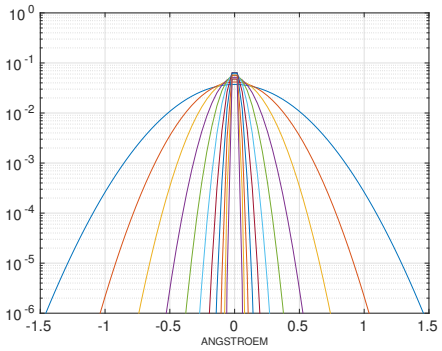
Singular values of side matrices for the long-range part $\mathbf{P}_l$ vs. N_0, $R_l = 12$.
Suits well for the C2T algorithm!

New range-separated tensor format

[Benner, Khoromskaia, Khoromskij, arXiv '16]

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

$$\mathbf{U} = \sum_{\nu=1}^{N_0} c_\nu \mathbf{U}_\nu, \quad \text{with} \quad rank(\mathbf{U}_\nu) \le R_0, \tag{5}$$

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

New range-separated tensor format

[Benner, Khoromskaia, Khoromskij '16]

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 $\mathrm{rank}(\mathbf{U}_0) \le R_0$,

$$\mathbf{A} = \sum_{k=1}^{R} \xi_k \mathbf{u}_k^{(1)} \otimes \cdots \otimes \mathbf{u}_k^{(d)} + \sum_{\nu=1}^{N_0} c_\nu \mathbf{U}_\nu, \quad \text{where} \quad \mathrm{diam}(\mathrm{supp}\mathbf{U}_\nu) \le 2\gamma. \tag{6}$$

Lemma

The storage cost of RS-canonical tensor is estimated by

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

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

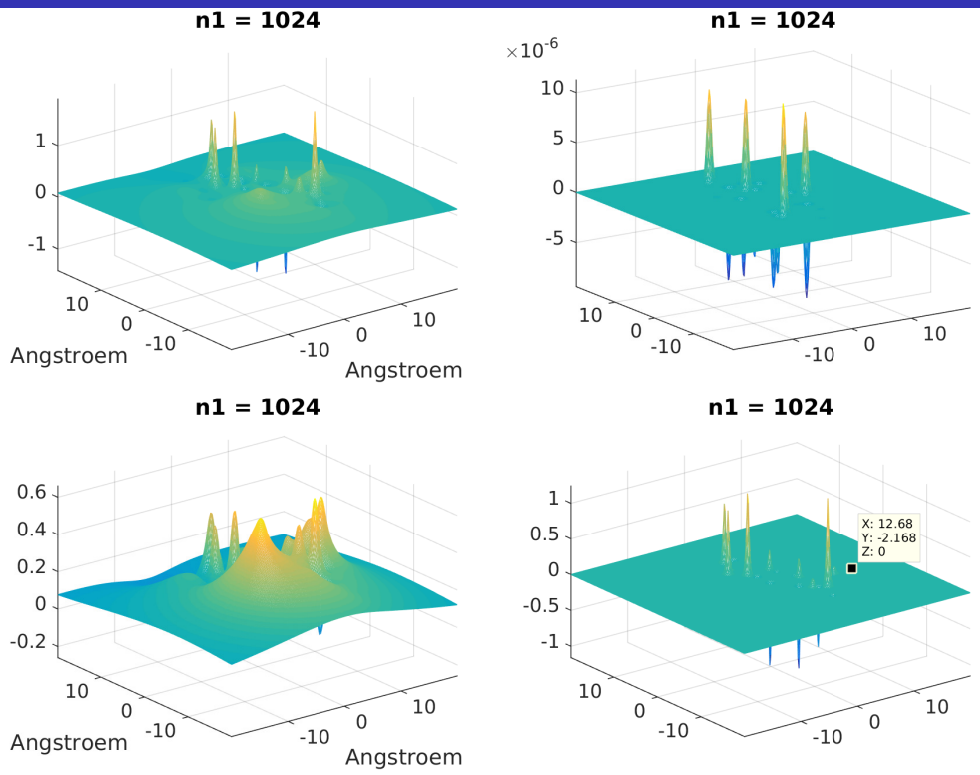


Figure : *Top: the potential sum at a middle plane of a cluster with 400 atoms (left), and the error of the RS-canonical approximation (right). Bottom: long-range part of a sum (left), short range part of a sum (right).*