MAX PLANCK INSTITUTE FOR DYNAMICS OF COMPLEX TECHNICAL SYSTEMS MAGDEBURG

CSC COMPUTATIONAL METHODS IN SYSTEMS AND CONTROL THEORY

IMPRS ProEng International Max Planck Research School for Advanced Methods in Process and Systems Engineering Magdeburg

Fast Solution of the Nonlinear Poisson-Boltzmann Equation Using the Reduced Basis Method and Range-Separated Tensor Format

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Electrostatic Interactions

The Poisson-Boltzmann equation (PBE) determines the electrostatic potential in a biomolecular system

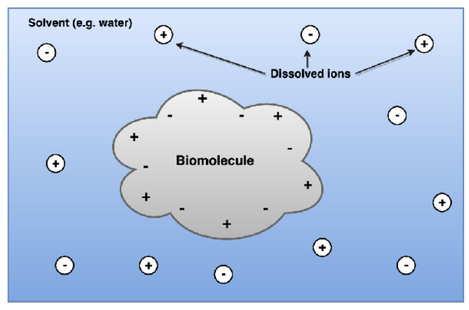


Figure 1: 2-D view of the 3-D Debye-Hückel model.

Mathematical Model

The traditional nonlinear PBE [3]:

$$-\vec{\nabla}.(\epsilon(x)\vec{\nabla}u(x)) + \bar{k}^2(x)\sinh(u(x)) = (\frac{4\pi e_c^2}{k_B T})\sum_{i=1}^{N_m} z_i\delta(x-x_i), \qquad x \in \mathbb{R}^3, \tag{1}$$

$$u(x) = (\frac{e_c^2}{k_B T})\frac{qe^{-k(d-a)}}{\epsilon_w(1+ka)d} \quad \text{on} \quad \partial\Omega, \quad d = |x - x_i|,$$

where

- $u(x) = \frac{e_c\psi(x)}{k_B T}$ - dimensionless potential,
- $k^2 = \frac{8\pi e_c^2 I}{1000\epsilon k_B T}$ - Debye screening constant,
- $C\sum_{i=1}^{N_m} z_i\delta(x-x_i)$ - molecular charge density,
- $I = \frac{1}{2}\sum_{i=1}^{N} c_i z_i^2$ - Ionic strength (parameter).

Canonical Tensor Approximation of the Newton Kernel

- Consider $\Omega = [-b, b]^3$, uniform n^3 rectangular grid Ω_n.
- Let $\psi_{\mathbf{i}}(\mathbf{x}) = \prod_{\ell=1}^{3}\psi_{i_\ell}^{(\ell)}(x_\ell)$ be a set of tensor-product basis functions.
- Discretize the Newton kernel $p(\|x\|) = \frac{1}{\|x\|}$ by its projection onto $\{\psi_{\mathbf{i}}\}$,

$$\mathbf{P} := [p_{\mathbf{i}}] \in \mathbb{R}^{n\times n\times n}, \quad p_{\mathbf{i}} = \int_{\mathbb{R}^3}\psi_{\mathbf{i}}(x)p(\|x\|)\,\mathrm{d}x.$$

- Low-rank canonical representation of $\mathbf{P}$ is based on exponentially convergent sinc-quadratures for the Laplace-Gauss transform of the Newton kernel

$$\frac{1}{\|x\|} = \frac{1}{\sqrt{\pi}}\int_{\mathbb{R}^+} e^{-t^2\|x\|^2}\mathrm{d}t = \frac{1}{\sqrt{\pi}}\int_{\mathbb{R}^+}\prod_{\ell=1}^{3} e^{-t^2(x_\ell)^2}\mathrm{d}t \approx \sum_{k=0}^{M} a_k e^{-t_k^2 z^2} \quad \|x\| > 0.$$

- The quadrature points and weights are $t_k = k\mathfrak{h}_M$, $a_k = a(t_k)\mathfrak{h}_M$, $\mathfrak{h}_M = C_0\log(M)/M$, $C_0 > 0$.
- Tensor $\mathbf{P}$ can be approximated by the separable R-term ($R = M+1$) canonical representation [4]

$$\mathbf{P} \approx \mathbf{P}_R = \sum_{k=0}^{M} a_k \bigotimes_{\ell=1}^{3}\mathbf{b}^{(\ell)}(t_k) = \sum_{k=0}^{M}\mathbf{p}_k^{(1)}\otimes\mathbf{p}_k^{(2)}\otimes\mathbf{p}_k^{(3)} \in \mathbb{R}^{n\times n\times n}.$$

Modified PBE by the Range-Separated (RS) Tensor format

Consider the free space electrostatic potential of (1) in form of Newton potential

$$u(x) = \frac{1}{\|x\|}, \quad x \in \mathbb{R}^3.$$

The RS canonical tensor format, developed and analyzed in [1], decomposes the Newton potential () into short- and long-range canonical tensor components

$$\frac{1}{\|x\|} \rightsquigarrow \mathbf{P}_R = \mathbf{P}_{R_s} + \mathbf{P}_{R_l}.$$

Discretize the exact equation for the Newton potential $-\Delta\frac{1}{\|x\|} = 4\pi\,\delta(x)$ using the finite difference method (FDM). This leads to the discrete representation of the Dirac delta

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

Split $\boldsymbol{\delta}_h$ into short- and long-range components, $\boldsymbol{\delta}_h = \boldsymbol{\delta}_s + \boldsymbol{\delta}_l$, we get

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

The solution to the modifed PBE is given by $u(x) = u^s(x) + u^r(x)$ such that $u^s(x) = \frac{1}{\|x\|^s} \rightsquigarrow \mathbf{P}_{R_s}$ and $u^r(x)$ is the solution to

$$\left.\begin{aligned} -\nabla\cdot(\epsilon\vec{\nabla}u^r(x)) + \bar{\kappa_2}^2(x)\sinh(u^r(x)) &= \delta_l, && \text{in } \Omega \\ u^r(x) &= \bar{\kappa_2}^2(x)\mathbf{P}_{R_l} && \text{on } \partial\Omega. \end{aligned}\right\} \tag{2}$$

Reduced Basis Method (RBM)

RBM algorithm for the modified PBE (2)

Algorithm 1 RBM algorithm

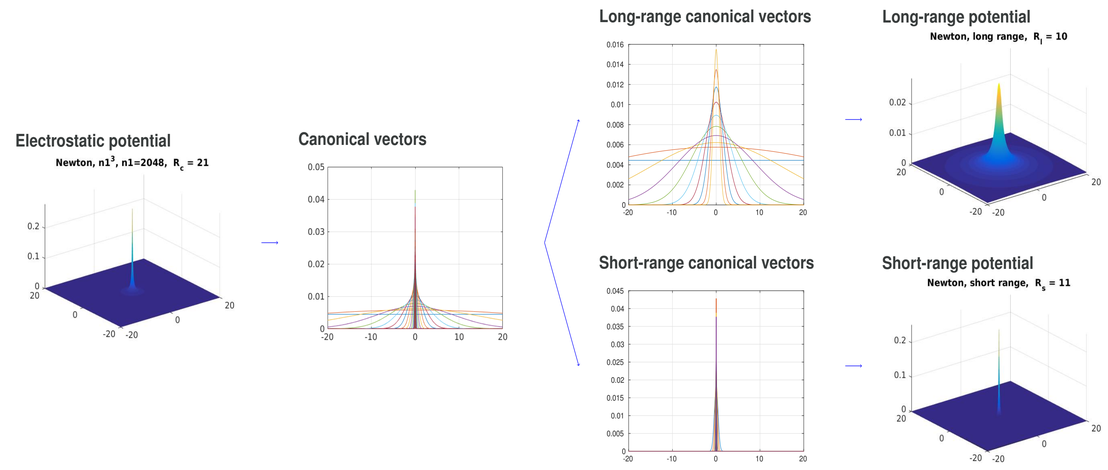
Input: System (2), tol, μ_1, n, training set ($\Xi \in D$).
Output: RB solution $u_{rb}(\mu)$, ROM, error estimator $\Delta(\mu)$.

1: Compute long-range solution to the linearized variant of (2) as the initial solution for Step 2.
2: Compute $u_l(\mu_n)$ to (2) for μ_n by AINSOLVE.
3: Set $\mathbb{V}_{rb} = \mathrm{span}\{u_\delta(\mu_1), \ldots, u_\delta(\mu_n)\}$.
4: Compute the reduced basis approximation $u_{rb}(\mu) \in \mathbb{V}_{rb}$ defined by $A_{rb}^\mu u_{rb}^\mu = f_{rb}^\mu$ by AINSOLVE, where $A_{rb}^\mu = \mathbb{V}_{rb}^T A_\delta^\mu \mathbb{V}_{rb}$ and $f_{rb}^\mu = \mathbb{V}_{rb}^T f_\delta^\mu$.
5: Evaluate the error estimator $\Delta(\mu)$.
6: Choose $\mu_{n+1} = \arg\max_{\mu\in\Xi}\Delta(\mu)$.
7: If $\Delta(\mu_{n+1}) \geq \mathrm{tol}$, then set $n := n+1$ and **go to Step 1**, otherwise **terminate**.

AINSOLVE is an accelerated inexact Newton solver which uses a preconditioned Krylov space to accelerate the convergence and avoids inversion of the Jacobian by excluding the Newton direction [2].

Numerical Results

RS canonical tensor format for the Newton potential



Accuracy of RS canonical tensor format for Poisson Equation (PE)

- Consider Acetazolamide compound with 18 atoms.
- Determine the error between the modified PE solution and the canonical solution.

n	97	129	257
Discrete L_2 norm	4.1176×10^{-7}	1.1936×10^{-7}	3.7003×10^{-9}

Table 1: The discrete L_2 norm of the error w.r.t. grid size.

Accuracy of the RB approximation for the modified PBE

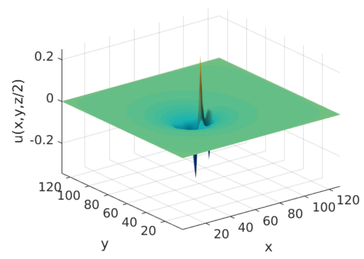
Cartesian grid properties and data

- Consider Acetazolamide compound,
- 129^3 grid and 32 Å box length,
- $\Xi \in D = [0.05, 0.15]$.

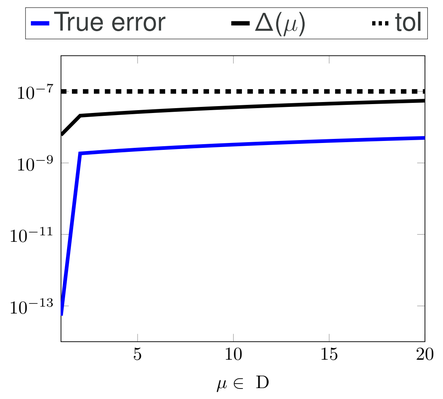
RB approximation properties

- Model reduction from $\mathcal{N}$ **= 2,146,689** to **N = 1**,
- Greedy tol (10^{-7}), sample size $\ell = 11$.

Runtime (seconds) and speed-up			
	FOM	ROM	Speed-up
Nonlinear system	4.174	5.785e-03	722



(a) RB approximation in the $\mathcal{N}$ space.



(b) Error estimator versus true error.

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[4] V. Khoromskaia and B. N. Khoromskij, *Grid-based lattice summation of electrostatic potentials by assembled rank-structured tensor approximation.*, Comp. Phys. Comm., 185 (2014).