Lectures on Tensor Numerical Methods for Multi-dimensional PDEs

Lect. 10-11. Bridging MLA with Scientific Computing: d-dimensional b.v. and spectral problems for Δ_d. Rank-structured eigenvalue problems. Stochastic PDEs. Parabolic problems in $\mathbf{d+1}$ *formulation*

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Outline of Lect. 10-11. Bridging MLA with Scientific Computing:

d-dimensional b.v. and spectral problems for Δ_d. Stochastic PDEs. Parabolic problems

1. Fast Poisson solver in $\mathbb{R}^d$ via low-rank *sinc* approximation of Δ^{-1}.
2. Iteration on subspace with rank truncation for eigenvalue problems.
3. Eigenvalue problems for rank-structured matrices: Reduced basis approach for the Bethe-Salpeter (BSE) equation.
4. Stochastic elliptic PDEs as parametric equations.
5. sPDEs in low-rank tensor formats by separation of spacial and parametric variables.
6. Preconditioned iteration in the CP format.
7. The QTT approximation of sPDE in 2D (log-additive case).
8. Simultaneous time-space discretization of parabolic equation in many dimensions. Rank estimates.
9. Numerical schemes and illustrations for the Fokker-Planck equation.
10. Chemical master equation for joint probability density of species in reaction channels.
11. Log-complexity in the discrete time via QTT approximation: long time dynamics.

PDES in $\mathbb{R}^d$. Tensor methods vs. challenges of the "curse of dimensionality": $N^d \to dN$

- Elliptic (parameter-dependent) BVP: Find $u \in H_0^1(\Omega)$, s.t.

$$\mathcal{H}u := -\operatorname{div}(a \operatorname{grad} u + u\mathbf{v}) + Vu = F \quad \text{in} \quad \Omega \in \mathbb{R}^d.$$

- Elliptic EVP: Find a pair $(\lambda, u) \in \mathbb{R} \times H_0^1(\Omega)$, s.t.

$$\mathcal{H}u = \lambda u \quad \text{in } \Omega \in \mathbb{R}^d, \quad \langle u, u \rangle = 1.$$

- Parabolic-type equations: Find $u : \mathbb{R}^d \times (0, T) \to \mathbb{R}$, s.t.

$$u(x, 0) \in H^2(\mathbb{R}^d): \quad \sigma \frac{\partial u}{\partial t} + \mathcal{H}u = F, \quad \sigma \in \{1, i\}.$$

- Large spacial/grid dimensions (grid-based methods in quantum chemistry):

$$\Omega = (-b, b)^d \in \mathbb{R}^d \ (d = 2, 3, ..., 100, ...): \ \text{large } N^d\text{-grids}, \ N = 2^L \sim 10^5.$$

- Multi-parametric (stochastic) equations:

$$a(y, x), \ F(y, x), \ u(y, x), \ y \in \mathbb{R}^M \ (M = 1, 2, ..., 100, ...).$$

- Long-time dynamics (TDHF, QMD, CME): $t = 0, t_1, t_2, ..., t_{N_t}, N_t = 2^Z$.
- Highly varying coeff. and rhs: Lattice systems, homogenization, interaction potentials.

Tensor numerical approximation to d-dimensional PDEs in $O(d)$-complexity

Traditional numerics meets tensor structures

- Numerical multi-linear algebra.
- Low-parametric separable approximation of d-variate functions (data compression).
- Low-rank tensor representation of linear operators: Green's functions(d), convolution(d), FFT(d), wavelet, multi-particle Hamiltonians, preconditioners.
- Iterative solvers to steady-state and temporal PDEs in "tensor formats".

Separation of variables beats the "curse of dimensionality"

- $O(dN)$-tensor numerical methods over $N \times N \times ... \times N$ grids: $N^d \to O(dN)$.

Super-compression

- $O(d \log N)$-Quantized tensor approximation (QCan, QTT, ...): $N^d \to O(d \log N)$.

Applications in higher dimensions

- d-dim. operators: Fast integration, convolution, Fourier and wavelet transforms.
- Electronic structure of molecules & crystals, quantum molecular dyn., M-particle interact.
- PDEs in $\mathbb{R}^d$: stochastic particle dynamics, stochastic PDEs, uncertainty quantification.

Low rank canonical approximation of Δ_d^{-1} (super-fast Poisson solver, preconditioning)

FEM d-Laplacian: $\Delta_d U = F$ on $N \times N \times \ldots \times N$ – grid in $\mathbb{R}^d$.

- $FFT_d = \bigotimes_{\ell=1}^{d} FFT_1$,
- $e^{-t\Delta_d} = \bigotimes_{\ell=1}^{d} e^{-t\Delta_1}$, $\Delta_1 = F_1^* \Lambda_1 F_1$, F_1 is the 1D sin-FFT.
- *sinc*-quadrature approx. $G_M \simeq G = {\Delta_d}^{-1}$ in the rank-R canonical format,

$$\Delta_d^{-1} = \int_0^\infty e^{-t\Delta_d} dt \simeq \sum_{k=-M}^{M} c_k \bigotimes_{\ell=1}^{d} \exp(-t_k \Delta_1) := \sum_{k=-M}^{M} c_k \bigotimes_{\ell=1}^{d} F_1^* e^{-t_k \Lambda_1} F_1 := G_M,$$

$$t_k = e^{k\mathfrak{h}}, \quad c_k = \mathfrak{h} t_k, \quad \mathfrak{h} = \pi/\sqrt{M},$$

with the exponential convergence rate in $R = 2M + 1$,

$$\left\| \Delta_d^{-1} - G_M \right\|_\infty \le C e^{-\pi\sqrt{M}}, \quad (\text{or} \quad \le C e^{-\pi M/\log M}).$$

N	Precomp	Time for sol	Residue	Relative L_2 error
2^8	6.14	2.98	6.6e-06	7.0e-06
2^9	8.37	3.52	8.7e-06	7.0e-06
2^{10}	10.81	4.02	9.4e-06	7.0e-06

100-d Poisson equation in C-QTT format, $F = 1$. $W = O(d|\log\varepsilon|^2 \log N)$ complexity.

Tensor-truncated iteration for boundary value problems (BVP)

Parametric elliptic BVP on nonlinear manifold $\mathcal{S}$:

$$\mathbb{A}(y)\mathbf{U}(y) = \mathbf{F}.$$

(A) Truncated preconditioned iteration:

$$\widetilde{\mathbf{U}}_{m+1} = \mathbf{U}_m - \mathbb{B}^{-1}(\mathbb{A}\mathbf{U}_m - \mathbf{F}), \quad \mathbf{U}_{m+1} := T_{\mathcal{S}}(\widetilde{\mathbf{U}}_{m+1}) \in \mathcal{S}.$$

(B) Direct minimization by ALS/DMRG iteration in TT/QTT formats:

$$\langle \mathbb{A}(y)\mathbf{U}(y) - \mathbf{F}, \mathbb{A}(y)\mathbf{U}(y) - \mathbf{F} \rangle \to \min.$$

Assumptions:

- $\mathbf{U}, \mathbf{F}$ allow the low $\mathcal{S}$-rank tensor approximation.
- Both $\mathbb{A}$ and $\mathbb{B}^{-1}$ have low-rank tensor decomposition in $\mathcal{S}$-format.
- Preconditioner $\mathbb{B}$ is spectral equivalent (close) to $\mathbb{A}$.

Good candidates for $\mathbb{B}^{-1}$:

(I) Shifted FD d-Laplacian inverse $(\Delta_d + aI)^{-1}$.

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

(II) $\mathbb{A}(y^*)^{-1}$.

Tensor-truncated power iteration: Eigenvalue problem for Laplacian

- **Elliptic EVP on nonlinear manifold $\mathcal{S}$:**
- Tensor truncated preconditioned inverse iteration.
- Tensor truncated Green function iteration.
- Minimization of the energy functional on $\mathcal{S}$.

Ex. 10.1. Find the minimal λ of $-\Delta_d u = \lambda u$ in $(0,\pi)^d$.

- Truncated inverse power iteration:

$$u_{n+1} = -\Delta_d^{-1} u_n, \qquad u_{n+1} = u_{n+1}/\|u_{n+1}\|.$$

Rank-$(2M+1)$, *sinc*-approximation of Δ_d^{-1}, $M = 49$ (see Lect. 8).
CPU time (sec.) per iteration (linear scaling in d).
$N_{iter} \le 6$.
$n^{\otimes d}$ grid points, $n = 2^9$.

d	Time/it	δ_λ-error	δ_u-error
3	0.9	$3.1 \cdot 10^{-6}$	$4.5 \cdot 10^{-4}$
10	2.9	$3.1 \cdot 10^{-6}$	$3.8 \cdot 10^{-4}$
50	14.7	$3.1 \cdot 10^{-6}$	$3.1 \cdot 10^{-4}$

Bethe-Salpeter eqn. (BSE): reduced basis approach by low-rank approximation

The BSE describes the excitation spectrum ω_n of molecules or solids.

- The 2×2-block matrix representation of BSE

$$F \begin{pmatrix} \mathbf{x}_n \\ \mathbf{y}_n \end{pmatrix} \equiv \begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} \mathbf{x}_n \\ \mathbf{y}_n \end{pmatrix} = \omega_n \begin{pmatrix} \mathbf{x}_n \\ \mathbf{y}_n \end{pmatrix}, \quad A, B \in \mathbb{R}^{N_{ov} \times N_{ov}}$$

$N_{ov} = N_o N_v = O(N_b^2)$, $N_v = N_b - N_o$, N_b is the size of GTO basis.

- The Tamm-Dancoff approximation (TDA) – symmetric spectral problem:

$$A\mathbf{u}_n = \mu_n \mathbf{u}_n.$$

- Eigenvalue solvers for J-symmetric (Hamiltonian) matrices: [Benner, Fassbender, Yang '15]

Numerical bottlenecks:

(A) Ab initio rank-structured representation of BSE matrix $\Rightarrow$
using factorization of TEI in molecular orbital basis, $\mathbf{B} \mapsto V \approx L_V L_V^T$.

(B) Central part of the spectrum is of interest $\Rightarrow$ using explicit F^{-1} (Sherman-Morrison).

(C) The system size $2N_{ov} \times 2N_{ov}$ may be huge, $2N_{ov} \in [10^3, 10^5] \Rightarrow$ QTT tensor approximation.

Prerequisites for generation of BSE matrix: ab initio Hartree-Fock calculus

Generating BSE matrices based on ab-initio Hartree-Fock calculations:

1. Full set of ground state energies (eigenvalues of the Hartree-Fock EVP)
$$\varepsilon_1, \ldots, \varepsilon_{N_b}.$$
2. The Galerkin coefficients in the expansion of molecular orbitals in GTO basis,
$$C = \{c_{\mu i}\} \in \mathbb{R}^{N_b \times N_b}.$$
3. TEI matrix $B = [b_{\mu\nu,\kappa\lambda}] \in \mathbb{R}^{N_b^2 \times N_b^2}$ via a low-rank Cholesky factorization,
$$B \approx LL^T, \quad L \in \mathbb{R}^{N_b^2 \times R_B}, \quad R_B = O(N_b)$$
presented in molecular orbitals basis,
$$B \mapsto V = [v_{ia;jb}] = L_V L_V^T, \quad L_V \in \mathbb{R}^{N_{ov} \times R_B}, \quad v_{iajb} = \sum_{\mu,\nu,\kappa,\lambda=1}^{N_b} C_{\mu i} C_{\nu a} C_{\kappa j} C_{\lambda b} b_{\mu\nu,\kappa\lambda}.$$

$i, j \in \mathcal{I}_o := \{1, \ldots, N_{orb}\}$ corresponds to occupied orbitals,
$a, b \in \mathcal{I}_v := \{N_{orb}+1, \ldots, N_b\}$ corresponds to virtual orbitals.

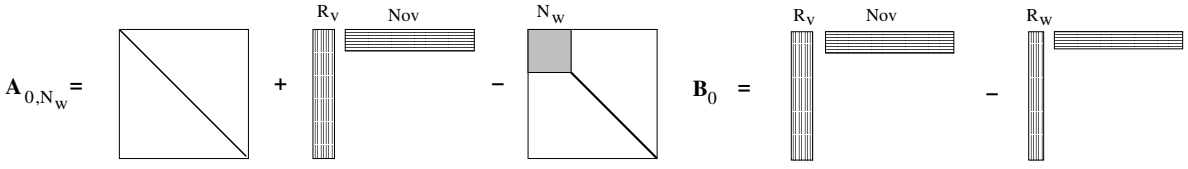
Simplified rank-structured problem and reduced basis approach

[Benner, Khoromskaia, BNK, Molec. Phys. '16]

Reduced basis approach: A and B are replaced by

$$A \mapsto A_0 := \mathbf{\Delta}\varepsilon + L_V L_V^T - \overline{W}_{N_W} \quad \text{and} \quad B \mapsto B_0 := L_V L_V^T - \widetilde{W}_r, \tag{1}$$

with $rank(\widetilde{W}_r) \le r$, and solve simplified problem.



Compute m_0 eigenpairs of (2), $\{(\mathbf{u}_n, \mathbf{v}_n)^T\} =: G_{m_0}$, of **the simplified structured problem**

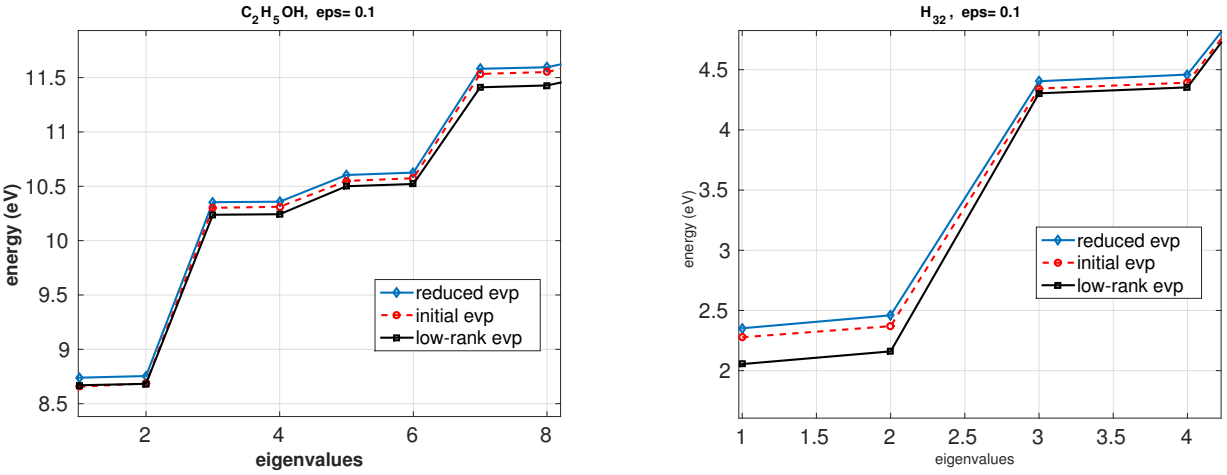
$$F_0 \begin{pmatrix} \mathbf{u}_n \\ \mathbf{v}_n \end{pmatrix} \equiv \begin{pmatrix} A_0 & B_0 \\ -B_0^* & -A_0^* \end{pmatrix} \begin{pmatrix} \mathbf{u}_n \\ \mathbf{v}_n \end{pmatrix} = \lambda_n \begin{pmatrix} \mathbf{u}_n \\ \mathbf{v}_n \end{pmatrix}. \tag{2}$$

Solve the reduced $m_0 \times m_0$ problem (direct diagonalization)

$$M_1 = G_{m_0}^T F_1 G_{m_0}, \quad S_1 = G_{m_0}^T G_{m_0} \in \mathbb{R}^{m_0 \times m_0},$$
$$M_1 \mathbf{y} = \gamma_n S_1 \mathbf{y}, \quad \mathbf{y} \in \mathbb{R}^{m_0}.$$

$\gamma_n \approx \omega_n$, $n = 1, \ldots, m_0$. Represent the first m_0 eigenvectors in the basis set $\{(\mathbf{u}_n, \mathbf{v}_n)^T\}$.

Surprising result I: Two-sided bounds for excitation energies (red. bl. $\overline{W}$)



Errors (in eV) for simplified and reduced BSE eigenvalues for Ethanol (C_2H_5OH) molecule and H_{32}-chain.

Lower bound is hard to prove: open question!

- Physical interpretation: open question!

Iterative solution of BSE using explicit Sherman-Morrison-Wudbury inverse

[Benner & Dolgov & Khoromskaia & BNK, '16]

- Compute eigenvalues with smallest magnitudes taking advantage from the rank-structured approximation of the matrix inverse A_0^{-1} and F_0^{-1}. Define

$$\begin{aligned} A_0 &= \boldsymbol{\Delta\varepsilon} + PQ^\top, & P &= \begin{bmatrix} L_V & L_W \end{bmatrix}, \quad Q = \begin{bmatrix} L_V & -L_W \end{bmatrix}, \\ B_0 &= \Phi\Psi^\top, & \Phi &= \begin{bmatrix} L_V & Y \end{bmatrix}, \quad \Psi = \begin{bmatrix} L_V & -Z \end{bmatrix}, \quad r = R_V. \end{aligned}$$

- Consider the Tamm-Duncoff approximation (TDA),

$$A_0\mathbf{x}_n = \mu_n\mathbf{x}_n, \quad \mathbf{x}_n \in \mathbb{R}^{N_{ov}} \quad A_0 \in \mathbb{R}^{N_{ov}\times N_{ov}}$$

Inverting a (block) diagonal plus low rank matrix: use the Sherman-Morrison formula for A_0^{-1}

$$A_0^{-1} = \boldsymbol{\Delta\varepsilon}^{-1} - \boldsymbol{\Delta\varepsilon}^{-1}P\left(I + Q^\top\boldsymbol{\Delta\varepsilon}^{-1}P\right)^{-1}Q^\top\boldsymbol{\Delta\varepsilon}^{-1}.$$

- The inner $2r \times 2r$ matrix

$$K = \left(I + Q^\top\boldsymbol{\Delta\varepsilon}^{-1}P\right)^{-1}$$

is small and can be computed explicitly at $\mathcal{O}(r^3 + r^2N_{ov})$ operations.

- Matrix-vector product $A_0^{-1}\mathbf{x}_n$ for the diagonal $\boldsymbol{\Delta\varepsilon}^{-1}$ and low-rank matrix in the second summand at the overall cost $\mathcal{O}(N_{ov}r)$.

Times: diagonal + low rank + reduced block

Times (s) for eig-solvers using reduced block representation of TDA and BSE systems.

Molecular syst.	H_2O	N_2H_4	C_2H_5OH	H_{32}	$C_2H_5NO_2$	H_{48}	$C_3H_7NO_2$
TDA size	180^2	657^2	1430^2	1792^2	3000^2	4032^2	4488^2
EIG(A_0)	0.02	0.5	4.3	9.8	37.6	91	127.4
TDA: EIGS(A_0)	0.09	0.33	2.8	0.77	16.1	3.0	30
TDA: EIGS(A_0^{-1})	0.07	0.09	0.25	0.77	0.54	3.0	1.0
BSE size	360^2	1314^2	2860^2	3584^2	6000^2	8064^2	8976^2
EIG(F_0)	0.08	4.2	33.7	68.1	274	649	903
BSE: EIGS(F_0^{-1})	0.21	0.37	1.11	1.10	2.4	2.92	4.6

Note: accuracy is better by the order of magnitude compared with diag + low-rank.

Time scales linearly in system size $O(N_{ov})$!

Surprising result II: Lower bound on the algebraic complexity of BSE, $\mathcal{O}(N_o^2)$

Usual relation: $N_b/N_o \geq C_{GTO} \approx 10$, i.e. $N_{ov} \approx C_{GTO} N_o^2$

$\Rightarrow$ quasi-optimal complexity of QTT solver

[Benner & Dolgov & Khoromskaia & BNK, '16]

Hypothesis: Estimate on the lower bound on the asymptotic algebraic complexity of the large scale BSE eigenvalue problem

$$\mathcal{W}_{BSE} = \mathcal{O}(\log(N_{ov}) r_{QTT}^2) = \mathcal{O}(\log(N_o) N_o^2).$$

Molecular syst.	C_2H_5OH	H_{32}	$C_2H_5\ NO_2$	H_{48}	$C_3H_7\ NO_2$
TDA size	1430^2	1792^2	3000^2	4032^2	4488^2
time QTT eig	0.14	0.23	0.32	0.28	0.63
abs. error (eV)	0.08	0.19	0.17	0.14	0.00034

Table: Time (s) and abs. error (eV) for QTT-DMRG eigensolvers for TDA.

Parametric Elliptic Problems: Stochastic PDEs

Find $u_M \in L^2(\Gamma) \times H_0^1(D)$, s.t.

$$\begin{aligned} \mathcal{A} u_M(y,x) &= f(x) \quad \text{in } D, \quad \forall y \in \Gamma, \\ u_M(y,x) &= 0 \qquad \text{on } \partial D, \quad \forall y \in \Gamma, \end{aligned}$$

$$\mathcal{A} := -\operatorname{div}\left(a_M(y,x)\operatorname{grad}\right), \quad f \in L^2(D), \quad D \in \mathbb{R}^d, \quad d = 1,2,3,$$

$a_M(y,x)$ is smooth in $x \in D$, $y = (y_1, ..., y_M) \in \Gamma := [-1,1]^M$, $M \leq \infty$.

Additive case (via the truncated Karhunen-Loéve expansion)

$$a_M(y,x) := a_0(x) + \sum_{m=1}^{M} a_m(x) y_m, \quad a_m \in L^\infty(D), \quad M \to \infty.$$

Log-additive case (more complicated)

$$a_M(y,x) := \exp(a_0(x) + \sum_{m=1}^{M} a_m(x) y_m) > 0.$$

- Sparse stochastic Galerkin/collocation: [Babuska, Nobile, Tempone '06-'10; Schwab el. '07-'10, Matthies '06]
- Stochastic Galerkin, canonical-$\mathcal{C}_R$ format, additive case: [BNK, Ch. Schwab, SISC, '10]
- QTT, both additive and log-additive cases: [BNK, Oseledets, CMAM, '10]

Stochastic collocation (additive case)

A parametric linear system, N - grid size in x (FEM, FD in x)

$$A(y)u(y) = f, \quad f \in \mathbb{R}^N, \; u(y) \in \mathbb{R}^N, \quad y \in \Gamma, \tag{3}$$

$$A(y) = A_0 + \sum_{m=1}^{M} A_m y_m, \quad A_m \in \mathbb{R}^{N \times N}, \quad \text{parameter dependent matrix.}$$

- Collocation on 1D grid, n - grid size in y_m, $m = 1, ..., M$

$$\{y_m^{(k)}\} =: \Gamma_n \in [-1,1], \quad k = 1, \ldots, n.$$

$\Rightarrow$ Assembled large linear system

$$\mathbb{A}\mathbf{u} = \mathbf{f}, \quad \mathbf{u}, \mathbf{f} \in \mathbb{R}^{Nn^M}, \quad \mathbb{A} \in \mathbb{R}^{Nn^M \times Nn^M},$$

$$\mathbb{A} = A_0 \times I \times \ldots \times I + A_1 \times D_1 \times I \times \ldots \times I + \ldots + A_M \times I \times \ldots \times D_M,$$

- D_m, $m = 1, \ldots, M$, is $n \times n$ diagonal matrix with positions of collocation points $y_m^{(k)} \in \Gamma_n$, on the diagonal.

$$\mathbf{f} = f \times e \times \ldots \times e, \quad e = (1, ..., 1)^T \in \mathbb{R}^n.$$

- Separation of x and $y_1, \ldots, y_M$ parameters: Kronecker rank $rank_{CP}(\mathbb{A}) \leq M$.

Preconditioned rank-truncated iteration in CP, TT, QTT

Given threshold $\varepsilon > 0$, iteration in canonical format:

$$\widetilde{\mathbf{u}}^{(k+1)} := \mathbf{u}^{(k)} - \omega \mathbb{B}_k^{-1} \left(\mathbb{A}\mathbf{u}^{(k)} - \mathbf{f} \right), \quad \mathbf{u}^{(k+1)} = T_\varepsilon(\widetilde{\mathbf{u}}^{(k+1)}) \to \mathbf{u},$$

T_ε is the rank truncation operator preserving accuracy ε.

- In additive case, $rank_{CP}(\mathbb{A}) \le M$.

A good choice of a (rank-1) preconditioner ($\mathbb{B}_0 = \mathbb{A}(y^*)$, $y^* = 0$)

$$\mathbb{B}_0^{-1} = A_0^{-1} \times I \times \ldots \times I.$$

- In log-additive case, adaptive preconditioner at iteration step k,

$$\mathbb{B}_k^{-1} = A(y_k^*)^{-1} \times I \times \ldots \times I,$$

$$y_k^* = \mathrm{argmin}_{QTT}(\|\mathbf{f} - \mathbb{A}\mathbf{u}^{(k)}\|).$$

Proven spectral equivalence, $\mathbb{B}_0 \sim \mathbb{A}$, in both cases.

In log-additive case, the rank estimate for $\mathbb{A}$ is a nontrivial task.

We have only local pointwise bound.

Numerics to sPDEs: additive case, canonical format

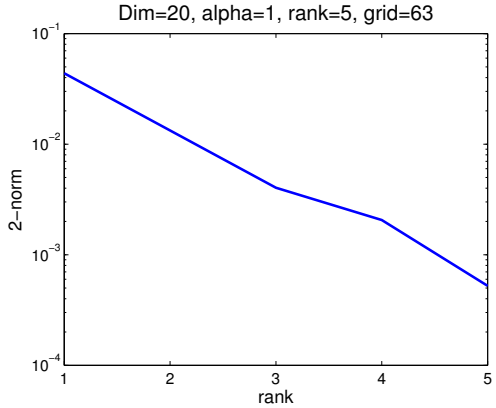
[BNK, Ch. Schwab, '10, SISC]

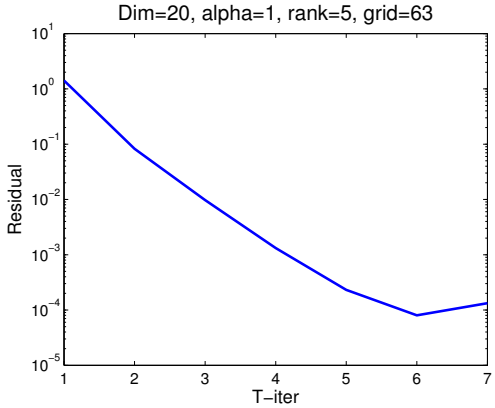
Preconditioned tensor-truncated iteration in $(d + M)$-dimensional parametric space.
Canonical format, $M \le 100$.

$\mathcal{S}$-truncated preconditioned iteration for solving sPDE $\mathbb{A}(y)\mathbf{u}(y) = \mathbf{f}$.

Choose $N^{\otimes(M+d)}$-grid, $d = 1$, $M = 20$ ($\mathcal{S} = \mathcal{C}_R$, $\mathbb{B}^{-1} := \mathbb{A}(0)^{-1}$).
Variable coefficients with exponential decay in KL-expansion ($N = 63$, $R \le 5$),

$$a_m(x) = 0.5\, e^{-m} sin(mx), \quad m = 1, 2, ..., M, \quad x \in (0, \pi).$$





Tensor-truncated preconditioned iteration scales linearly in M.

Matrix ranks: QTT-rank/both cases

[BNK, Oseledets, '10, CMAM] Stratified 2D-dimensional sPDE in the two cases:

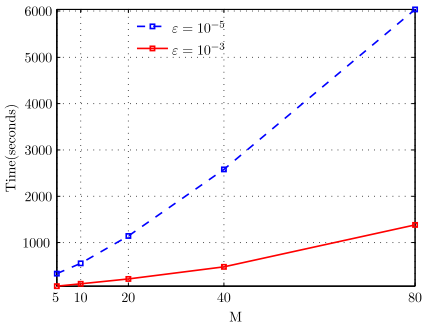
1. Polynomial decay: $a_m(x) = \frac{0.5}{(m+1)^2} \sin mx_1$, $x_1 \in [-\pi, \pi]$, $m = 1, \ldots, M$.
2. Exponential decay: $a_m(x) = e^{-0.7m} \sin mx_1$, $x_1 \in [-\pi, \pi]$, $m = 1, \ldots, M$.

The param. space is discretized on a uniform 2^p-mesh, $p = 8$, in $[-1, 1]^M$ in each mode.

M	QTT-rank(10^{-7})	QTT-rank(10^{-3})
5	33	11
10	43	21
20	51	23
40	50	25

QTT-rank of the matrix: 2D SPDE, log-additive case, exponential decay, grid $N = 128$.

Time vs. M.



Time dependent problems: dynamics on tensor manifold

▶ Parabolic BVP projected onto $\mathcal{S} \subset \mathbb{V}_{\mathbf{n}}$: $\mathbf{U} \in \mathcal{S}$,

$$\sigma \frac{\partial \mathbf{U}}{\partial t} - \mathbb{H}\mathbf{U} = \mathbf{F}, \quad \mathbf{U}(0) = T_{\mathcal{S}}\mathbf{U}(0), \quad \sigma = 1, i.$$

Problem 1. Complex-time molecular Schrödinger eq. in QMD,

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

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

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

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

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

Problem 3. Chemical master equation. Joint probability density $\mathcal{P}(\mathbf{x}, t)$,

$$\mathcal{P}(\mathbf{x}, 0) = \mathcal{P}_0, \quad \frac{d\mathcal{P}(\mathbf{x}, t)}{dt} = \mathbf{A}\mathcal{P}(\mathbf{x}, t), \quad \mathbf{x} \in \mathbb{R}^{n_1 \times \ldots \times n_d}.$$

Main approaches: overview

- **Time integrators**
  - Sparse grids in (x, t): [Schwab et al.; Griebel et al.]
  - Dirac-Frenkel projection onto Tucker/TT/QTT-manifold $\mathcal{S}$,

$$\langle \frac{dy}{dt} - Hy, \delta y \rangle = 0, \quad \delta y \in T_y \mathcal{S}.$$

    [Meyer et al. '03; Lubich '07-'12; BNK, Oseledets, Schneider '12]
  - Greedy iterations (canonical format)
    [Cancés, Le Brie, Lelievre, Maday et al; Chinesta et al; Suli et al; Binev, Cohen, Dahmen, et al]
  - Time stepping by implicit scheme + TT/QTT + ALS/DMRG local solver,
    [Dolgov, BNK, Oseledets '11]
- **Global time-space schemes: all-at-ones solvers in d + 1**
  - Global time-space separation by QTT-Cayley transform [Gavrilyuk, BNK '11]
  - QTT-Tucker + ALS-type solver on global (x, t) tensor manifold [Dolgov, BNK '12-'13]

QTT-Cayley transform method

Dynamics and spectrum of high-dimensional Hamiltonians [Gavrilyuk, BNK '11]

$$\psi(t) = \sum_{p=0}^{\infty} L_p^{(0)}(t) u_p \equiv i(H + iI)^{-1} \sum_{p=0}^{\infty} L_p^{(0)}(t) T^p \psi_0,$$

$T = T(H) = H(H + iI)^{-1}$ is the Cayley transform, u_p can be found by the recursion

$$u_0 = i(H + iI)^{-1} \psi_0,$$
$$u_{p+1} = H(H + iI)^{-1} u_p, \quad p = 0, 1, ...$$

- The m-term truncated series representation

$$\psi_m(t) = \sum_{p=0}^{m} L_p^{(0)}(t) u_p. \tag{4}$$

Def. 10.2. $f = \sum a_k \varphi_k(x)$ is called H-analytic if there is $C = C(f) > 0$, s.t.

$$\|H^n f\| = \sqrt{\sum_{k=0}^{\infty} a_k^2 \lambda_k^{2n}} \leq C^n n! \quad \text{for all} \quad n = 1, 2, 3, ...$$

where $\{\varphi_k, \lambda_k\}$ is the spectral data of H.

Complexity bounds, spectral calculus

Lem. 10.1. Let ψ_0 be H-analytic, then for every fixed $s > 0$, s.t. $\|\psi_0\|_{s,H} := \sum_{k=0}^{\infty} \frac{s^k}{k!} \|H^k \psi_0\| < \infty$, the $\psi_m(t)$ converges exponentially in m,

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

where c, c_1 are positive constants independent of m.

Lem. 10.2. QTT-rank of $U = [\psi_m(t_k)]_{k=1}^N$, $t_k = k\Delta t$, is bounded by

$$rank_{QTT}(U) \le \sum_{p=0}^{m} (p+1) rank_{QTT}\, T^p(\psi_0).$$

For the harmonic oscillator: $rank_{QTT}(U) \le C m^2 rank_{QTT}(\psi_0)$.

- The *energy spectrum* is recovered by FFT of autocorrelation function

$$a(t) = \langle \psi_m(t), \psi(0) \rangle = \sum_{p=0}^{m} L_p^{(0)}(t) \langle u_p, \psi_0 \rangle, \quad G(E) = \int_0^{\infty} a(t) e^{iEt} dt.$$

- Simultaneous time-space QTT decomposition of complexity

$$O(\log N_t \log N\, m^4\, (rank_{QTT}\, T^m(\psi_0))^2).$$

Numerics: High-dimensional spectral calculation in QMD

- The complexity of one step is linear in d, logarithmic in 1D grid-size and polynomial in QTT-ranks of the wave function. MD with Henon-Heiles potential [BNK, Oseledets '11]

$$H = -\Delta_d + V; \quad V(\mathbf{q}) = \sum_{k=1}^{d} q_k^2 + \text{cubic term}.$$

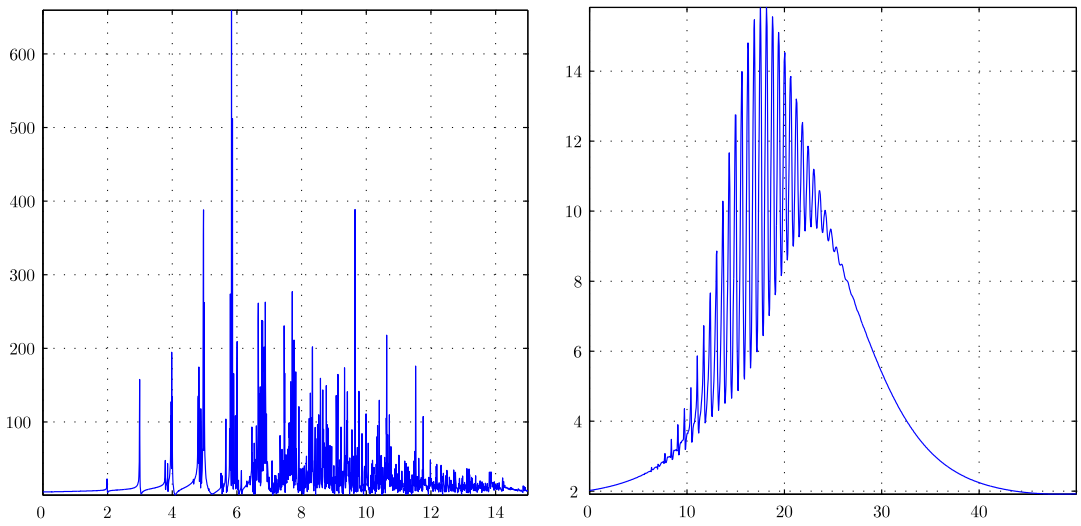


Figure: Spectrum of Henon-Heiles Hamiltonian ($d = 4, 10$), QTT-rank truncation.

The Fokker-Planck equation

Real-time evolution. The Fokker-Planck equation.

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

where $\psi : \mathbb{R}^d \to \mathbb{R}$, and $v : \mathbb{R}^d \to \mathbb{R}^d$ is a given field.

Time propagation scheme with tensor truncation

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

Examples of the time-propagator S:

$S = I - \tau A$ (explicit Euler),

$S = (I + \tau A)^{-1}$ (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, $\psi_k \to \psi_*$ (normalized *probability density* ψ_*),

$$A\psi_* = 0, \quad \int \psi_* dx_1 \dots dx_d = 1.$$

Discretization on global QTT-tensor manifold in space-time

Crank-Nikolson, A, f_k are given in the TT or QTT format,

$$(I + \frac{\tau}{2}A)y_{k+1} = (I - \frac{\tau}{2}A)y_k + \frac{\tau}{2}(f_k + f_{k+1}). \tag{5}$$

(A) Time stepping by DMRG iteration for $(I + \frac{\tau}{2}A)y_{k+1} = F_{k+1}$.

(B) Global block solver in TT/QTT format. Rewrite (5):

$$y_{k+1} - y_k + \frac{\tau}{2}Ay_{k+1} + \frac{\tau}{2}Ay_k = \frac{\tau}{2}(f_k + f_{k+1}).$$

All-at-ones solver: Solve the huge global $N^d \times N_t$ system in QTT format [Dolgov, BNK, Oseledets, '11]

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

Global $O(\log N_x \log N_t)$ block-AMEn solver in QTT-Tucker format, [Dolgov, Savostianov '13]

Discretization in space

A uniform $N \times ... \times N$ tensor grid in $[-a, a]^d$ with $N = 2^L$.

$$A \approx \Delta_d + T, \quad T = C_1\Lambda_1 + C_2\Lambda_2 + \ldots + C_d\Lambda_d,$$

$C_\ell\Lambda_\ell$ is the discretization of the term

$$\frac{\partial}{\partial x_\ell}(v_\ell\psi_\ell),$$

and v_ℓ is the ℓ-the component of the vector field v,

$$\Lambda_\ell(i_1, \ldots, i_d, i_1, \ldots, i_d) = v_\ell(x(i_1), x(i_2), \ldots, x_d(i_d)).$$

C_ℓ is a matrix of central-difference operator in the ℓ-th mode,

$$C_\ell = I \otimes \ldots \otimes \underbrace{C}_{\ell} \otimes \ldots \otimes I, \quad C = \frac{1}{h}\texttt{triadiag}[-1, 0, 1].$$

Approximation order $O(h^2)$ in both time and space: $h \approx \tau$.

Model problem

The *dumbbell model* discretized on large grids.

$$v = Kq + \mathrm{grad}(\varphi),$$

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

The potential energy φ is given as

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

The following functional of the solution is interesting:

$$\tau(t) = \int \psi(t)\,(q \otimes \mathrm{grad}(\varphi))\,dq.$$

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

The *dumbbell model* discretized on large grids.

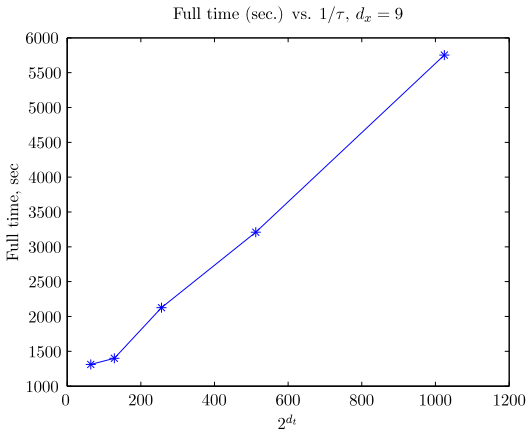


Figure: TT-solution time vs. τ, $N_x = 2^{d_x}$, $N_t = 2^{d_t}$, *Time* $= O(r^2 N_t N_x)$.

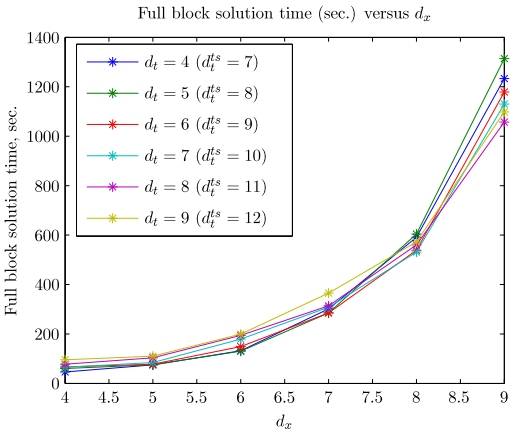


Figure: Block QTT-solution time vs. d_t, d_x, $r = O(\log N_x)$, *Time* $= O(r^2 \log N_t \log N_x)$.

[Dolgov, BNK, Oseledets '11]

Chemical master equation (CME): High-dimensional real-time dynamics

▶ **QTT-Tucker for chemical master equation:**

Species $S_1, ..., S_d$ react in M channels.
The vector of concentration $\mathbf{x} = (x_1, ..., x_d)$, $x_i \in \{0, ..., N_i - 1\}$,
The stoichiometric vector $\mathbf{z^m} \in \mathbb{Z}^d$,
The propensity function $w^m(\mathbf{x}), m = 1, ..., M$.
CME is a deterministic difference equation on the joint probability density $P(x, t)$:

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

$w^m = \{w^m(\mathbf{x})\}$ and $P(t) = \{P(\mathbf{x}, t)\}$, $\mathbf{x} \in \bigotimes_{i=1}^{d} \{0, \ldots, N_i - 1\}$,

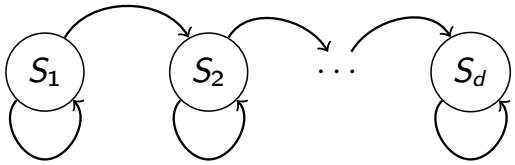
$$\mathbf{J^z} = J^{z_1} \otimes \cdots \otimes J^{z_d},$$

$$J^z = \begin{bmatrix} \mathbf{0} & \cdots & \mathbf{1} & & \\ & \ddots & & \ddots & \\ & & \ddots & & \mathbf{1} \\ & & & \ddots & \vdots \\ & & & & \mathbf{0} \end{bmatrix} \begin{matrix} \\ \\ \leftarrow \text{ row } N - z, \\ \\ \leftarrow \text{ row } N \end{matrix} \quad \text{if } z \geq \mathbf{0}; \qquad J^z = (J^{-z})^\top, \text{ if } z < \mathbf{0}.$$

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

[Dolgov, Khoromskij, NLLA '13]

Figure: Cascade signaling network



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

δ_m is the m-th identity vector.

Problem size is huge: 64^{20}

Convergence history

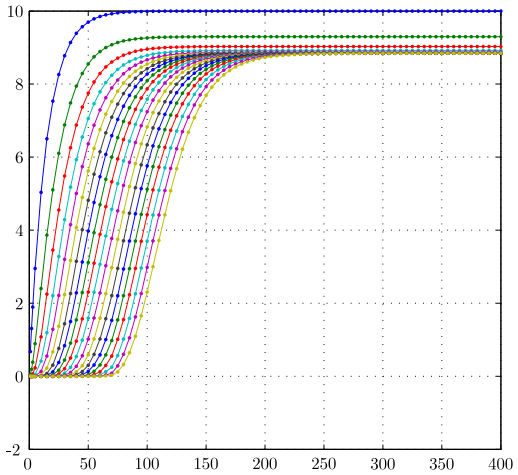


Figure: **Mean concentrations** $\langle x_i \rangle(t)$.

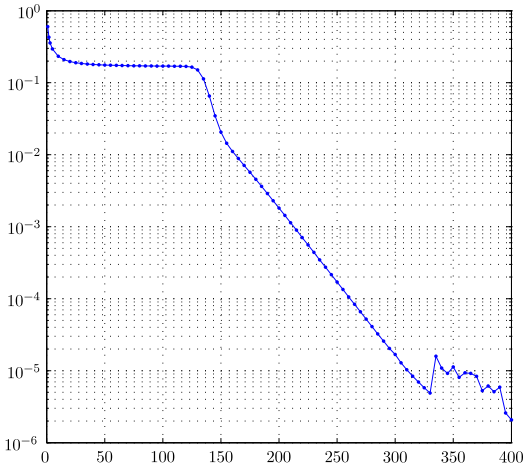


Figure: **Closeness to the kernel** $\dfrac{||AP||}{||P||}(t)$

$O(\log N_t)$ CPU time

The performance of the global state-time scheme vs.

- numbers of time steps N_t in each interval $[(p-1)T_0, pT_0]$.
- the time interval widths T_0

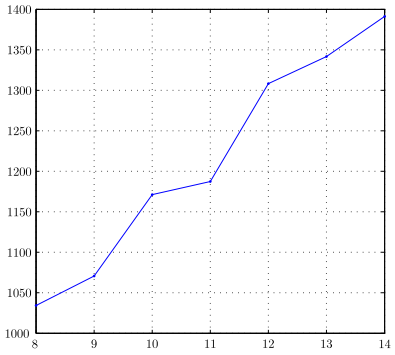


Figure: CPU time (sec.) versus $\log_2(N_t)$, $T_0 = 15$.

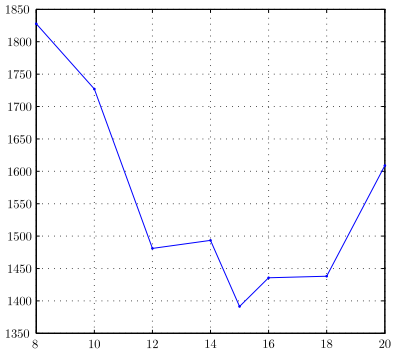


Figure: CPU time (sec.) versus T_0, $N_t = 2^{14}$.

- Logarithmic complexity in N_t.
- There is an optimal time-step T_0.