Outline of Lecture 4 (I).

1. High-dimensional boundary-value problems:

Parametric and stochastic PDEs.

2. Eigen-value problems:

Spectrum of the d-Laplacian and the Hartree-Fock eq. (QTT version).

3. Time dependent problems in higher dimensions:

Spectrum of the molecular Hamiltonian and the Fokker-Planck eq.

4. Conclusions.

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

(A) Truncated preconditioned iteration:

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

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

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

Assumptions:

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

Applications: Stochastic PDEs, preconditioning.

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

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

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

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

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

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

- Sparse stochastic Galerkin/collocation: **[Babuska, Nobile, Tempone '06-'10; Schwab el. '07-'10]**
- Stochastic Galerkin, $\mathcal{C}_R$ form., additive case: **[BNK, Ch. Schwab, SISC, '10]**
- HT, additive case: **[Kressner, Tobler, '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)

$$A(y)u(y) = f, \quad f \in \mathbb{R}^N, \; u(y) \in \mathbb{R}^N, \quad y \in \Gamma, \tag{1}$$

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

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

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

$\Rightarrow$ 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: $rank_C(\mathbb{A}) \le M$.

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

[BNK, Ch. Schwab '10, SISC] 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, a good choice of a (rank-1) preconditioner

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

In log-additive case, adaptive preconditioner at iter. step k,

$$\mathbb{B}_k^{-1} = A(y_k^*)^{-1} \times I \times \ldots \times I, \quad y_k^* = \text{argmin}_{QTT}(\|\mathbf{f} - \mathbb{A}\mathbf{u}^{(k)}\|).$$

Note: $\mathbb{B}_0$ corresponds to $y^* = 0$.

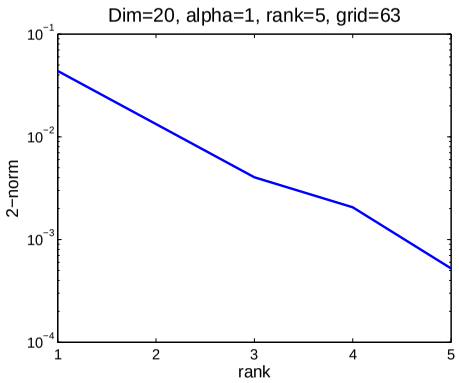
Proven spectral equivalence, $\mathbb{B}_0 \sim \mathbb{A}$, in both cases.

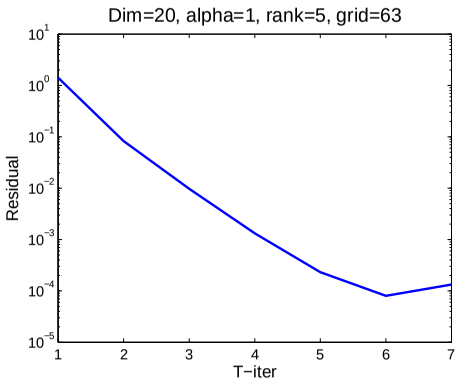
[BNK, Ch. Schwab, '10, SISC]

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

$\mathcal{S}$-truncated preconditioned iteration for solving sPDE
$N^{\otimes(M+d)}$-grid, $d = 1$, $M = 20$ ($\mathcal{S} = \mathcal{C}_R$, $\mathbb{B}^{-1} := \mathbb{A}(0)^{-1}$).
Variable coefficients with exponential decay ($N = 63$, $R \leq 5$),

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





- Smooth and random coefficient in y.

$$a(y,x) = a(y) := 1 + \sum_{m=1}^{M} a_m y_m \quad \text{with} \quad \gamma = \|\mathbf{a}\|_{\ell_1} := \sum_{m=1}^{M} |a_m| < 1, \tag{2}$$

for the truncated sequence of (spatially homogeneous) coefficients $a_m = (1+m)^{-\alpha}$, $(m = 1, ..., M)$ with algebraic decay rates $\alpha = 2, 3, 5$

The zero order sPDE,

$$a(y)u(y) = f. \tag{3}$$

Highly oscillating random coefficient

$$a(y) = 1 + \sum_{m=1}^{M} a_m y_m \, H(y_m - c_m(y_m)),$$

the pwc function $c_m(y_m)$, given by a random n-vector at $[-1, 1]$.

$H : \mathbb{R} \to \{-1, 1\}$, $H(x) = -1$ for $x < 0$, and $H(x) = 1$ for $x \geq 0$.

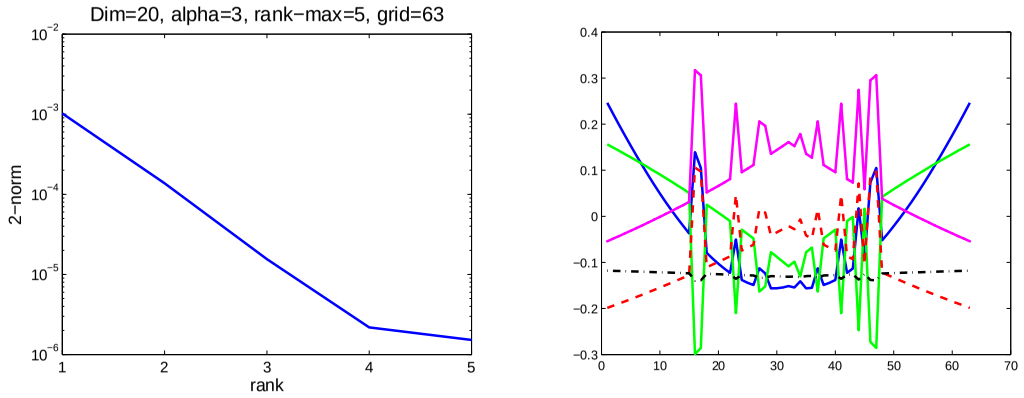


Figure 1: Approximation error vs. rank R (left) and the five canonical vectors in variable y_1 (right) for the solution of (3), $M = 20$.

r-convergence exponential, same as in the smooth case.

The canonical vectors – highly oscillating.

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

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

The parametric space is discretized on a uniform mesh in $[-1, 1]$ with 2^p points in each spatial direction, $p = 8$.

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

Table 1: QTT-rank of the matrix, 2D SPDE, log-additive case, exponential decay $N = 128$.

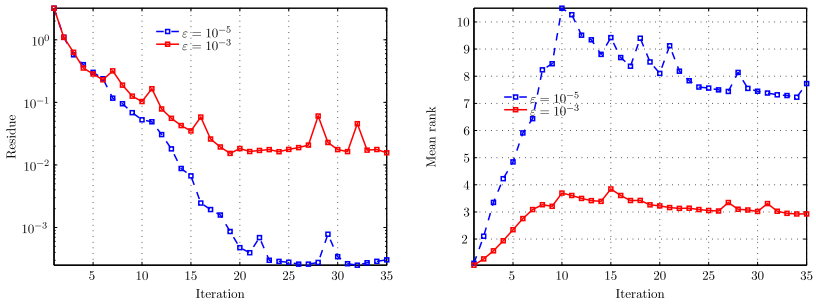
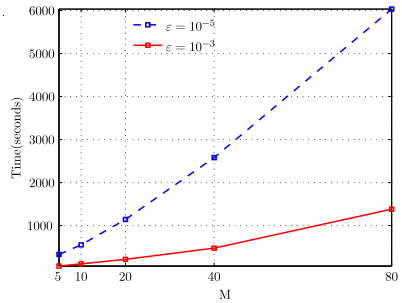


Figure 2: Convergence in the stratified 2D example with two different truncation parameters, 1-point preconditioner, Left: Residue with iteration, Right: Ranks with iteration



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

Ex. 3. Truncated inverse power iter. [Hackbusch, BNK, Sauter, Tyrtyshnikov '09]:

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

n^d grid points, $n = 2^9$. Rank-$(2M+1)$, $sinc$-appprox. of Δ_d^{-1}, $M = 49$.

The CPU time (sec.) per iter. (linear scaling in d). $N_{iter} \le 6$.

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	$3.1 \cdot 10^{-6}$	$3.1 \cdot 10^{-4}$

Objectives in Many-particle models.

- The electronic Schrödinger eq. for many-particle system in $\mathbb{R}^d$,

$$\mathbf{H}\Psi = \Lambda\Psi$$

with the Hamiltonian $\mathbf{H} = \mathbf{H}[r_1, ..., r_{N_e}]$,

$$\mathbf{H} := -\frac{1}{2}\sum_{i=1}^{N_e}\Delta_i - \sum_{a=1}^{K}\sum_{i=1}^{N_e}\frac{Z_a}{|r_i - R_a|} + \sum_{i<j\le N_e}\frac{1}{|r_i - r_j|} + \sum_{a<b\le K}\frac{Z_a Z_b}{|R_a - R_b|},$$

Z_a, R_a are charges and positions of the nuclei, $r_i \in \mathbb{R}^3$.

Hence the problem is posed in $\mathbb{R}^d$ with high dimension $d = 3N_e$, where N_e is the (large) number of electrons.

Desired size of the system is $N_e = O(10^q)$, $\quad q = 1, 2, 3, 4, ...?$

Proteins: $q = 3, 4$.

Molecular dynamics, electronic structure calculations for small molecules: $q = 1, 2$.

- Hartree-Fock equation

$$\left[-\frac{1}{2}\Delta - V_c(x) + \int_{\mathbb{R}^3} \frac{\rho(y)}{\|x-y\|} dy\right] \phi_i(x) - \frac{1}{2}\int_{\mathbb{R}^3} \frac{\tau(x,y)}{\|x-y\|}\phi_i(y)dy = \lambda\phi_i(y),$$

over $\phi_i \in H^1(\mathbb{R}^3)$, $\int_{\mathbb{R}^3} \phi_i\phi_j = \delta_{ij}$, $1 \le i,j \le N_e$.

$\tau(x,y) = \sum_{i=1}^{N_e} \phi_i(x)\phi_i(y)$ - electron density matrix,

$\rho(x) = \tau(x,x)$ - electron density,

$\frac{1}{\|x\|}$ - Newton kernel,

V_c - external potential with singularities at centers of atoms.

Tensor-structured nonlinear DIIS iteration

[Khoromskaia, BNK, Flad, SISC '11]

▷ Tucker and QTT representation of operators (e.g., 3D convolution).

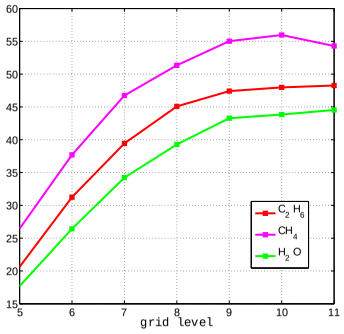
▷ Multigrid tensor iterations on large $N \times N \times N$ grids.

▷ CPU time scales linearly or even logarithmically in the grid size N.

[Khoromskaia, BNK, Schneider, '11]

N	128	256	512	1024
$1/\|x\|$	13.8	16.0	17.5	18.0
$\rho(x)$	32.0	40.0	45.8	48.6
$V_H = \rho * \frac{1}{\|x\|}$	32.1	34.9	20.2	28.2

Table 2: QTT-ranks of projected $1/\|x\|$, $x \in \mathbb{R}^3$, the Hartree pot. V_H, electron density ρ of CH_4.



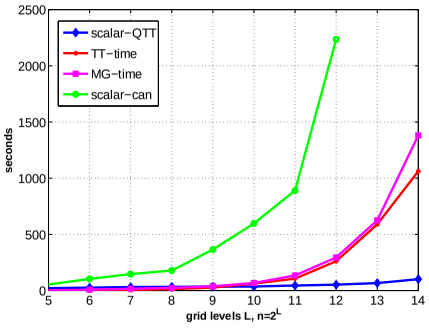


Figure 3: Average QTT-ranks for CH_4, C_2H_6, H_2O vs. levels L, $N = 2^L$, $\epsilon = 10^{-6}$ (left). Comparative timing for $\langle V_H g_k, g_m\rangle$, max grid $2^{42} \approx 10^{12}$ (right).

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

$$\sigma \frac{\partial \mathbf{U}}{\partial t} - \mathbb{A}\mathbf{U} = 0, \quad \mathbf{U}(0) = T_{\mathcal{S}}\mathbf{U}(0), \quad \sigma = 1, i. \tag{4}$$

▶ Time integrators

(a) Sparse grids in (x,t): [Schwab, Stivenson et al.; Griebel et al.; Suli et al.]

(b) Dirac-Frenkel projection onto $\mathcal{S}$, [Meyer et al '03, Lubich '07, Schneider '11]

(c) Implicit Euler/CN, global $(x.t)$ in QTT/DMRG [Dolgov, BNK, Oseledets '11]

▶ Global time-space separation by QTT-Cayley transform [Gavrilyuk, BNK '11]

Ex. 5. Time-dependent molecular Schrödinger eq. in QMD,

$$i\frac{\partial \psi}{\partial t} = H\psi = (-\frac{1}{2}\Delta_d + V)\psi, \quad \psi(x,0) = \psi_0(x), \quad x \in \mathbb{R}^d, \tag{5}$$

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

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

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

where $T = T(H) = H(H+iI)^{-1}$, and u_p can be found from 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

$$\psi_m(t) = \sum_{p=0}^{m} L_p^{(0)}(t) u_p. \tag{6}$$

Def. 3. $f = \sum a_k \phi_k(x)$ is called H-analytic if there is $C = C(f) > 0$, s.t.

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

where $\{\phi_k, \lambda_k\}$ is the eigendata of H.

Lem. 5. Let ψ_0 be H-analytical, 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, ε are positive constants independent of m.

Lem. 6. 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

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

- Discretize on tensor grid in a spatial box $[-a, a]^d$.

$$\Delta_d = \Delta_1 \otimes I \otimes \ldots \otimes I + \ldots + I \otimes \ldots \otimes \Delta_1, \quad rank_{QTT}(\Delta_d) = 4.$$

Discrete time propagation by

$$e^{iH\tau} \approx S := e^{i\Delta_d \frac{\tau}{2}} e^{iV\tau} e^{i\Delta_d \frac{\tau}{2}}, \quad e^{i\tau\Delta_d} = \bigotimes_{k=1}^{d} e^{i\tau\Delta_1}, \tag{7}$$

$$\psi_{k+1} = \psi(t_{k+1}) = T_\varepsilon(S\psi(t_k)), \quad t_k = k\Delta t.$$

$e^{iV\tau}$, is represented by cross QTT-approximation, if tensor is given as an elementwise function of a QTT-tensor.

- Autocorrelation function

$$a(t) = \langle \psi(t), \psi(0) \rangle, \quad 0 \le t \le T.$$

- The complexity of one step is linear in d, logarithmic in 1D grid-size and polynomial in QTT-ranks of the wavefunction.

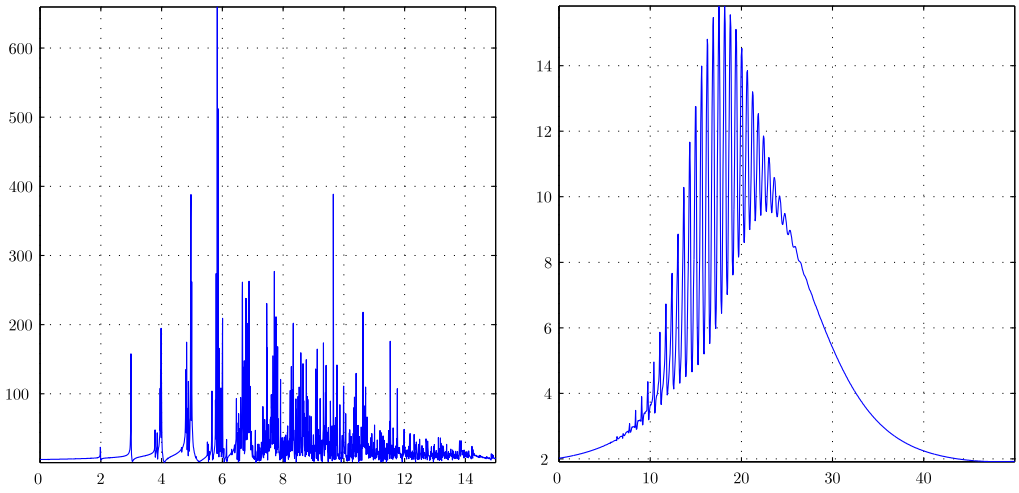


Figure 4: Spectrum of Henon-Heiles Hamiltonian ($d = 4, 10$), QTT-rank truncation.

[BNK, Oseledets '11]

Ex. 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:
$S = (I + \tau A)^{-1}$ (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*),

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

[Dolgov, BNK, Oseledets '11]

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

$$(I + \frac{\tau}{2}A)y_{k+1} = (I - \frac{\tau}{2}A)y_k + \frac{\tau}{2}(f_k + f_{k+1}). \qquad (8)$$

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

(B) Global block solver in TT/QTT format. Rewrite (8):

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

Solve the huge global $N^d \times N_t$ system in QTT format:

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

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 op. 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 $O(h^2)$.

The *dumbbell model* discretized on large grids.

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

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

The potential energy ϕ is given as

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

The following functional of the solution is interesting:

$$\tau(t) = \int \psi(t) \left(q \otimes \mathrm{grad}(\phi)\right) dq.$$

In particular, we test

$$\eta(t) = -\frac{\tau_{12}}{\beta}, \quad \Psi(t) = -\frac{\tau_{11} - \tau_{22}}{\beta}.$$

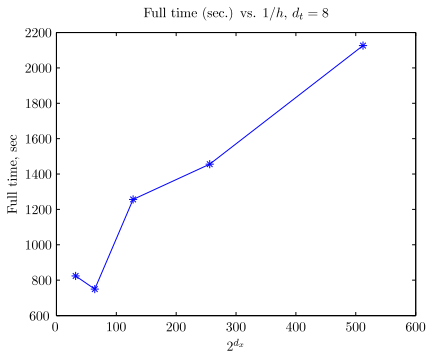


Figure 5: Full solution time (sec.) versus h in the dumbbell case

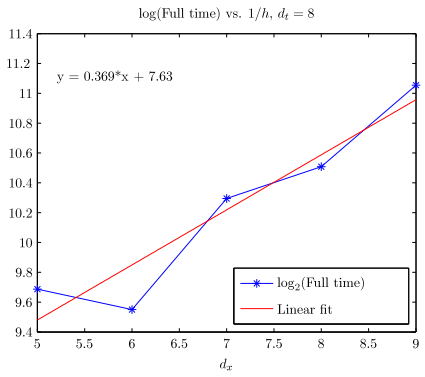


Figure 6: Full sol. time in log-scale vs. h, dumbbell case, TT format

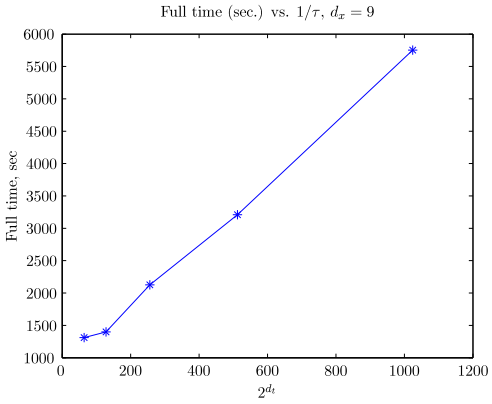


Figure 7: Full solution time versus τ, TT format.

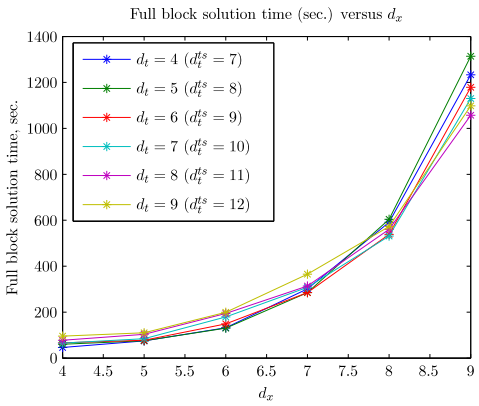


Figure 8: Full block sol. time vs. d_t and d_x, QTT, $O(\log N_t \log^3 N_x)$.

Challenging problems:

QTT-FFT & QTT-convolution in $O(d \log N)$ complex. $(+)$,

Stochastic/parametric PDEs $(\pm)$,

Electronic Schrödinger hamiltonians, DFT $(\mp)$,

Molecular Schrödinger eq., $i\frac{\partial}{\partial t} + \mathcal{H}$, PES $(\pm)$.

Lecture notes on tensor numerical methods [BNK '10]:

http://www.math.uzh.ch/fileadmin/math/preprints/06_11.pdf

More details:

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

Collaborations:

MPI MiS, Leipzig; INM, Moscow (GERRUSLAB);
TU Berlin; ETH/Uni. Zürich

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