Approximating Eigenpairs in Quantum Chemistry

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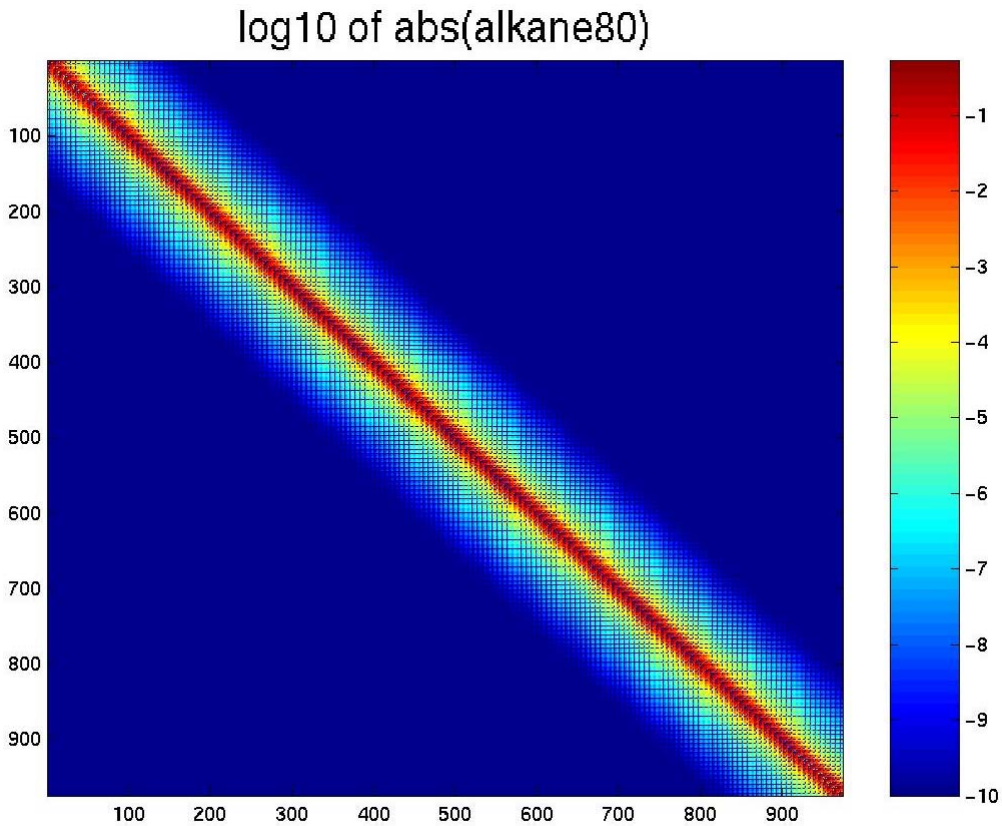
Outline

- Introduction, problem statement
- Framework: Approximation levels
- D&C (tridiagonal/block-tridiagonal)
- Analysis and experimental results
- Summary and outlook

Introduction

Central Problem I

- Given: Symmetric matrix $A \in \mathbb{R}^{n \times n}$, preferably "diagonally heavy"



Central Problem II

- Given: Symmetric matrix $A \in \mathbb{R}^{n \times n}$ (preferably "diagonally heavy"), tolerance parameter τ
- Wanted: *Approximate* spectral decomposition $A \approx \hat{V} \hat{\Lambda} \hat{V}^T$, s.t.

$$\| A - \hat{V} \hat{\Lambda} \hat{V}^T \| \leq \tau \quad \text{and} \quad \| \hat{V}^T \hat{V} - I \| \leq \varepsilon_{\text{mach}}$$

  - Essentially the full spectrum required

Application: Quantum Chemistry

- Quantum-mechanical equations for many-electron systems (non-relativistic time-independent Schroedinger Equation)
- *Restricted Closed-Shell Hartree-Fock Approximation*
- Linearization: expand unknown molecular orbitals into finite series of basis functions

Application: Quantum Chemistry

- Construct the *Fock matrix F* and the *Overlap matrix S* $\Rightarrow$
- *Roothaan Equations* (nonlinear eigenvalue problem):

$$\mathbf{F(C)\ C = S\ C\ E}$$

- Self-consistent-field (SCF) procedure $\Rightarrow$ sequence of (generalized) linear eigenproblems

Application: Quantum Chemistry

- Objective:
  - Develop efficient *approximate* linear eigensolver for use in SCF procedure
- Desirable properties ("wish list"):
  - Variable accuracy parameter
  - Efficiency
  - Parallelization

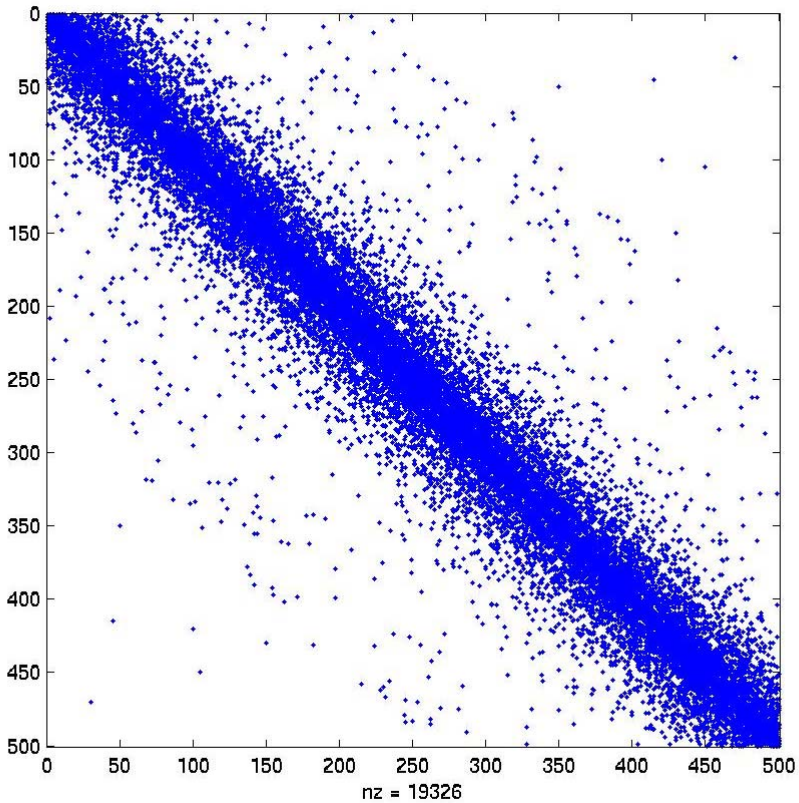
Approximation Levels

3 Levels of Approximation

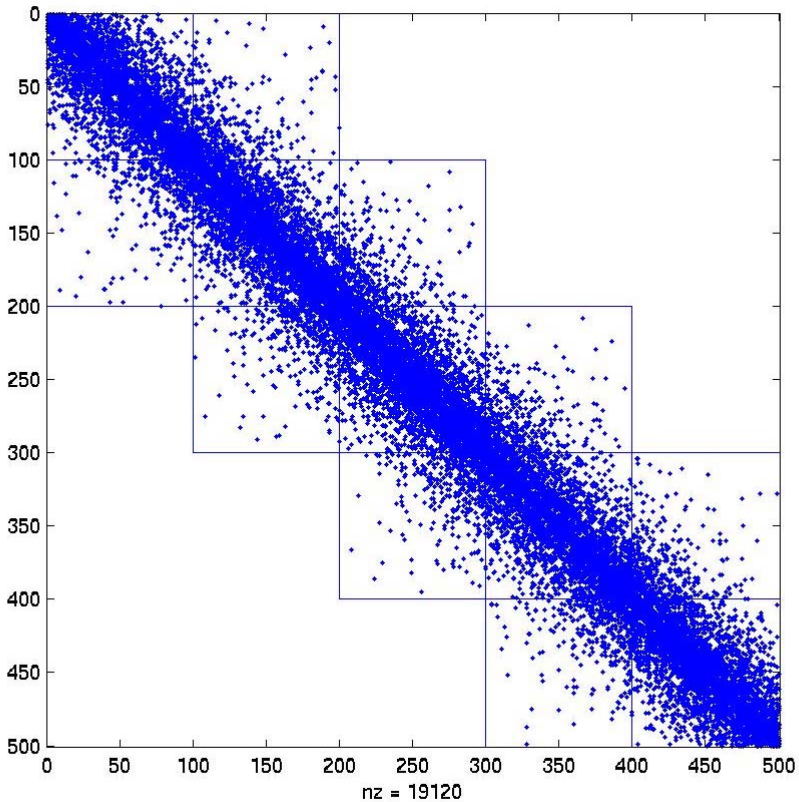
- Approximate A by a symmetric block-tridiagonal matrix B.

  (thresholding, reordering, bandwidth reduction,...)

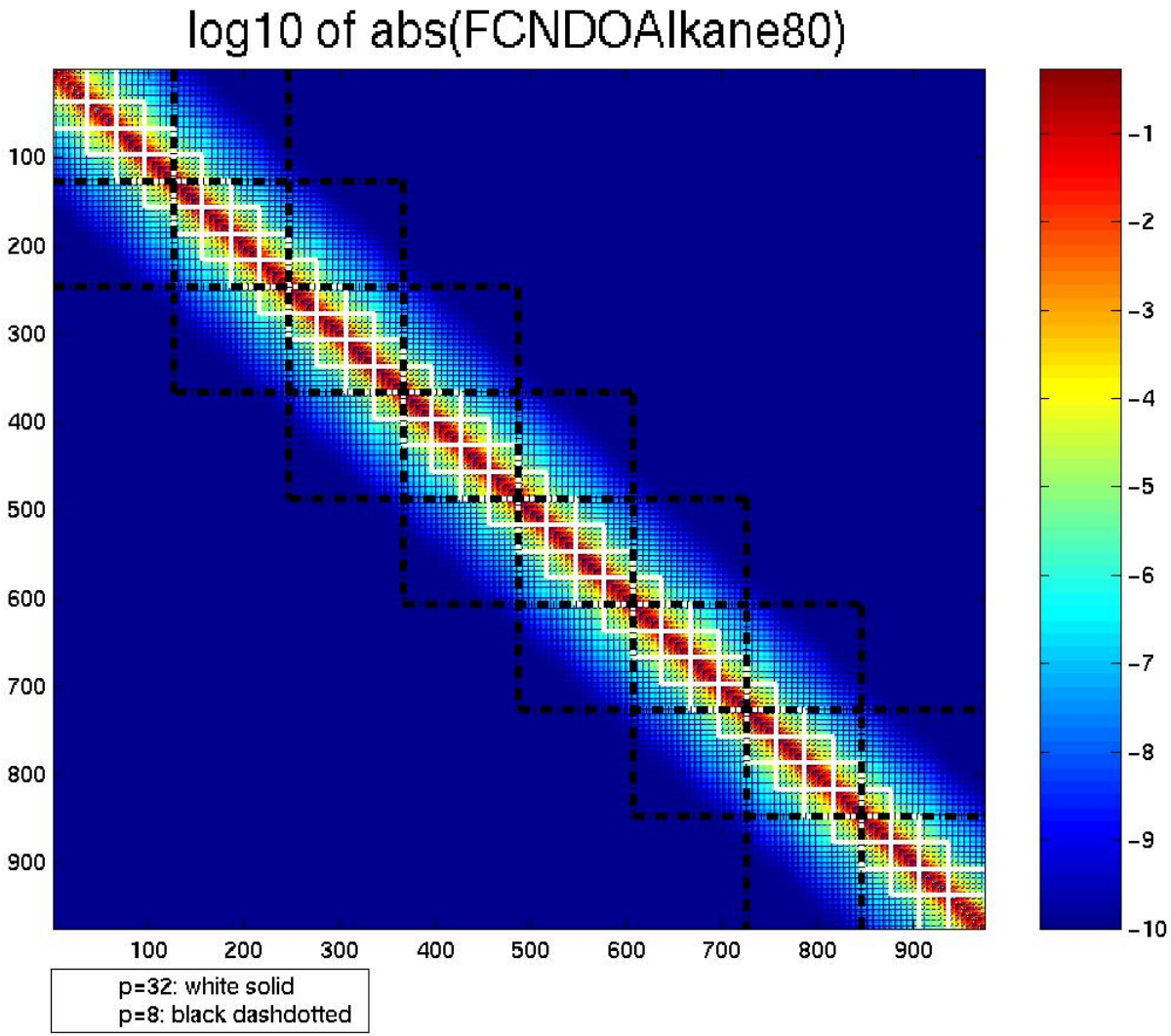
Original Matrix



Block-Tridiagonal Approximation B



QC Linear Alkane: alkane80



Approximation Error I

- Error caused by thresholding and reordering can be bounded

$$|\alpha_i - \beta_i| \leq n\tau_1$$

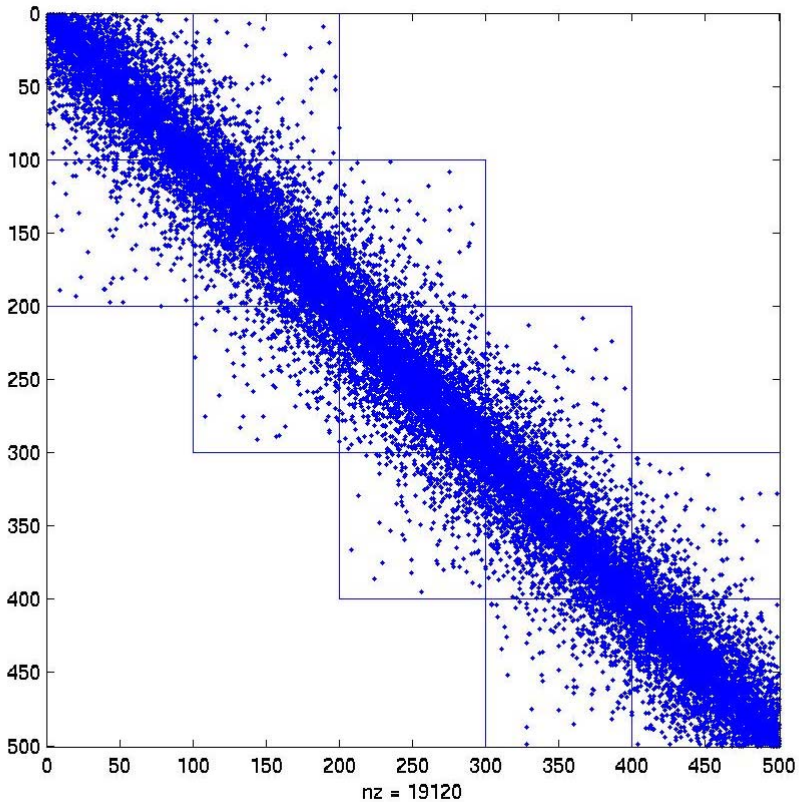
where α_i...eigenvalues of A
β_i...eigenvalues of B
τ_1 ...thresholding tolerance

3 Levels of Approximation

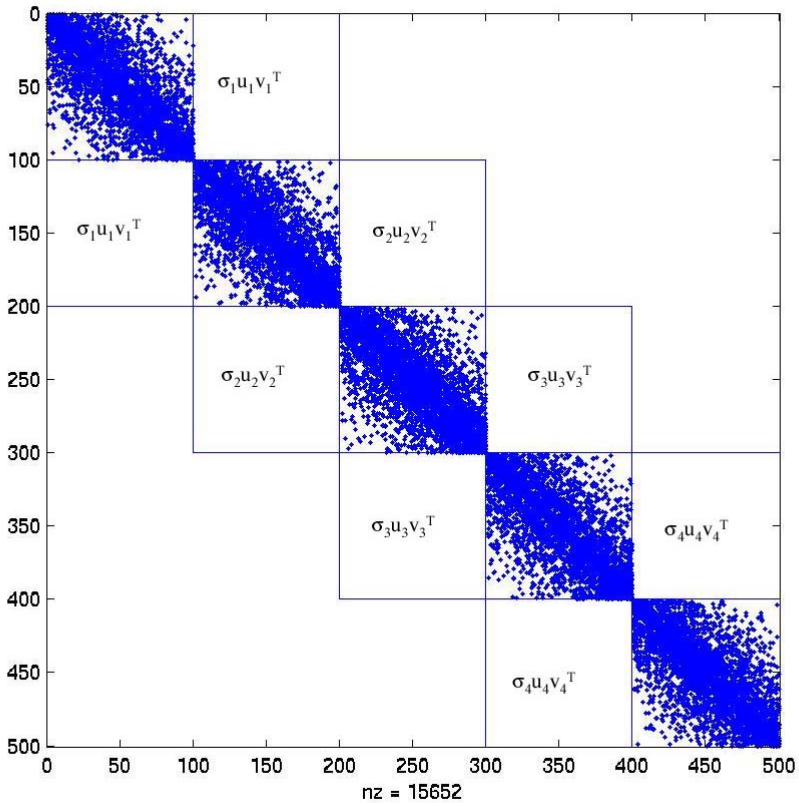
- Approximate A by a symmetric block-tridiagonal matrix B.
- Approximate the off-diagonal blocks of B by low(er) rank matrices (→ B').

  (SVD-based rank-r_i approximations)

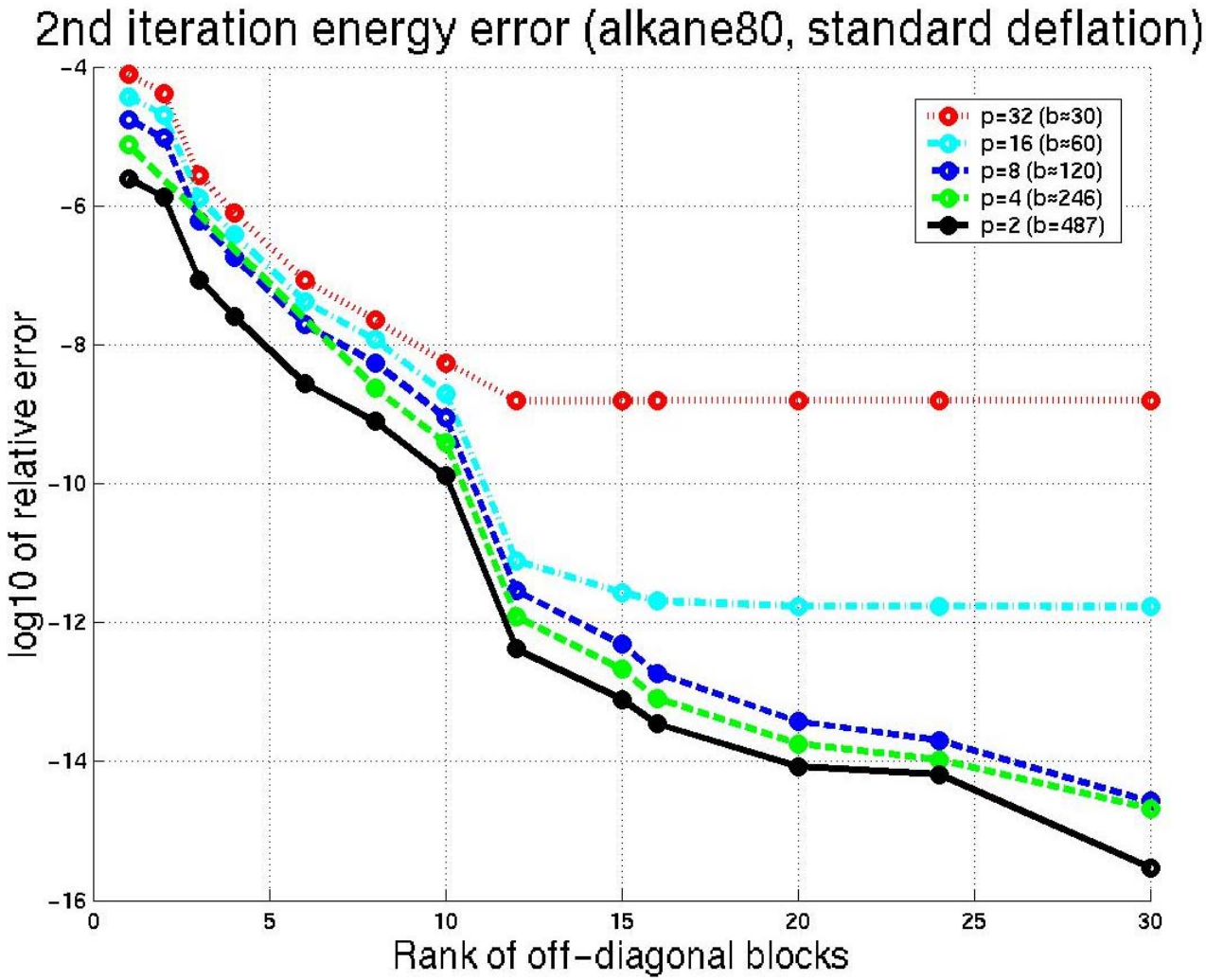
Block-Tridiagonal Approximation B



Rank-1 Approximation of Off-Diagonal Blocks



Relative Errors in 2nd Iteration Energy



Approximation Error II

- Error caused by rank approximation of off-diagonal blocks can be bounded as

$$| \beta_i - \lambda_i | \leq 2\sqrt{n} \max_{k=1,2,\ldots,p-1} \sum_{j=r_k+1}^{m_k} \sigma_j^k$$

where β_i ...eigenvalues of B
λ_i ...eigenvalues of B′
(approximated blocks)
σ_j^k ...j-th singular value of the k-th subdiagonal block

3 Levels of Approximation

- Approximate A by a symmetric block-tridiagonal matrix B.
- Approximate the off-diagonal blocks of B by low(er) rank matrices (→ B′).
- Apply (approximative) block divide-and-conquer algorithm to B′.

  (relaxed deflation,…)

Divide-and-Conquer for *Tridiagonal* Problems

[Golub (1973); Bunch et al. (1978); Cuppen (1981); Dongarra & Sorensen (1987); Gu & Eisenstat (1994/1995); Tisseur & Dongarra (1999);…]

Divide-and-Conquer

Transform - Solve - Back-Transform
Transform - Solve - Back-Transform

Split

.
.
.

Synthesize

Transform - Solve - Back-Transform

Tridiagonal Divide-and-Conquer

- Central task:

  Eigenvalues and -vectors of a rank-one modification problem

$$D + xx^T$$

  with a diagonal matrix D

Deflation

$$D + xx^T$$

- Zero component $x_i = 0 \Rightarrow$ corresponding eigenpair is known explicitly
- Multiple entry $d_i \Rightarrow$ corresponding eigenpairs can be computed cheaply
- Problem size can be reduced *(deflated)*
- Cost for eigenvector update is reduced (block structured eigenvector matrix)

Tridiagonal D&C

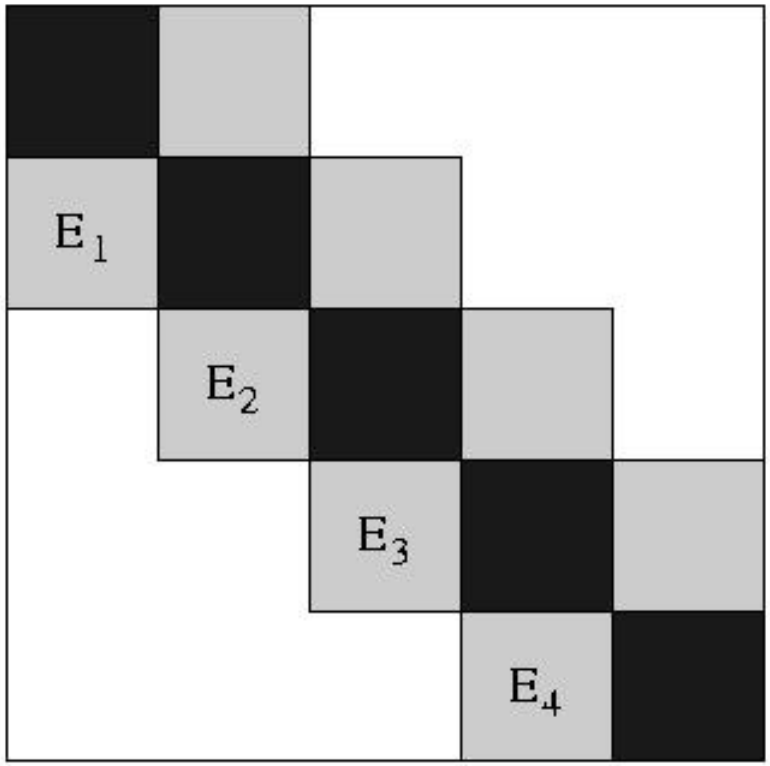
- Accumulation (multiplication) of eigenvector matrices
- Theoretical arithmetic complexity:

$$c\tfrac{4}{3}n^3 + O(n^2) \text{ flops}$$

- In practice often lower due to deflation
- One of the fastest algorithms available

(*Approximative*) Divide-and-Conquer for *Block-Tridiagonal* Matrices

Block-Tridiagonal D&C



$$E_i = \sum_{j=1}^{r_i} \sigma_j^i u_j^i v_j^{iT}, \; i = 1, 2, \ldots, p-1$$

- Subdivision (p blocks):
  - SVDs (off-diagonal)
  - Corrections and eigendecompositions (diagonal blocks)
- Synthesis:
  - r_i rank-one modifications per off-diagonal block
  - Best merging order: lowest rank last

Relaxed Deflation

- Standard deflation tolerance (LAPACK):

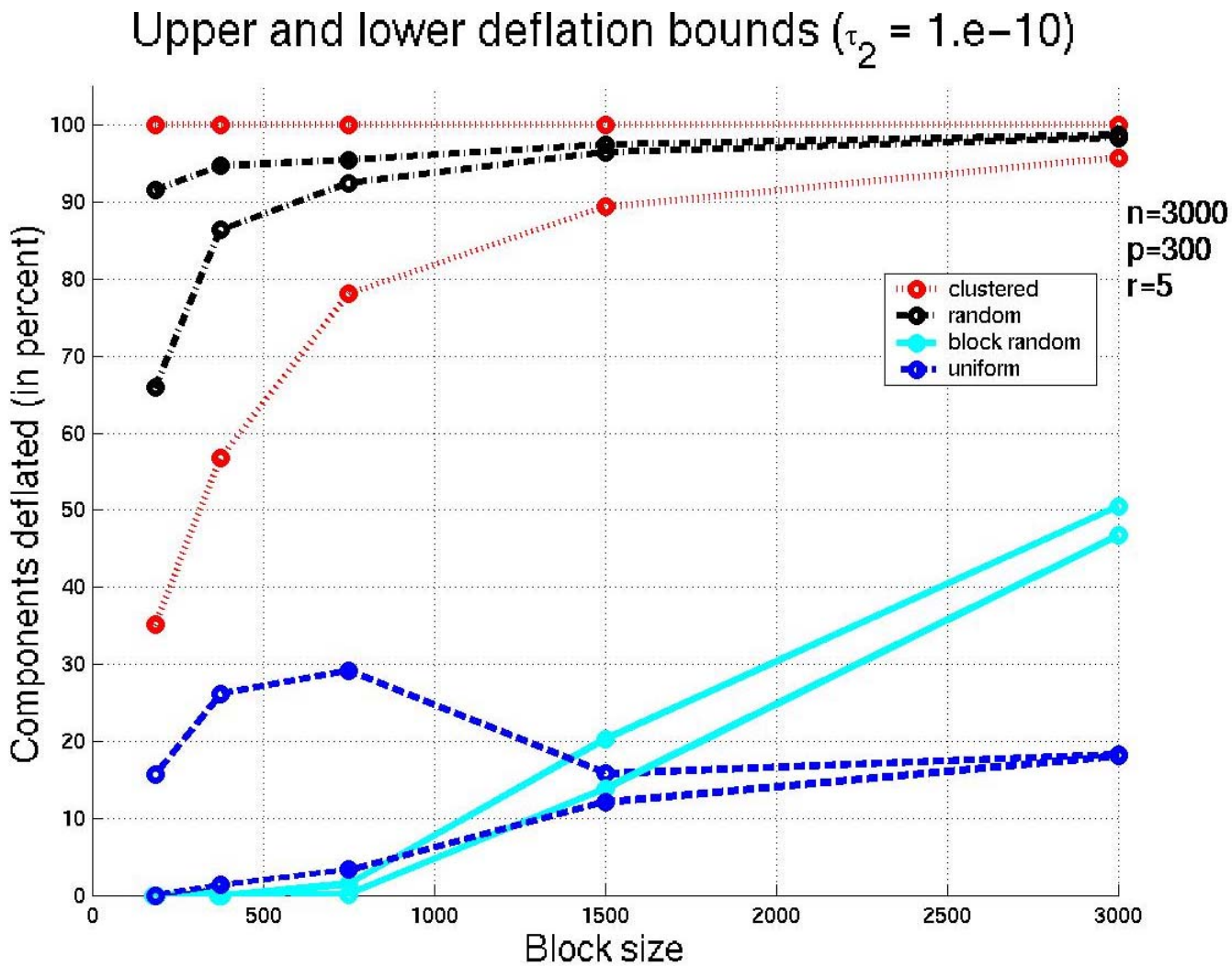
$$\tau_L := c\varepsilon \left\| B' \right\|$$

- Relaxed deflation tolerance $\tau_2 < \tau_L$
  - Absolute eigenvalue error proportional to τ_2
  - Allows for (potentially) much more deflation
  - Significant computational savings
  - Very attractive if medium/low accuracy is sufficient

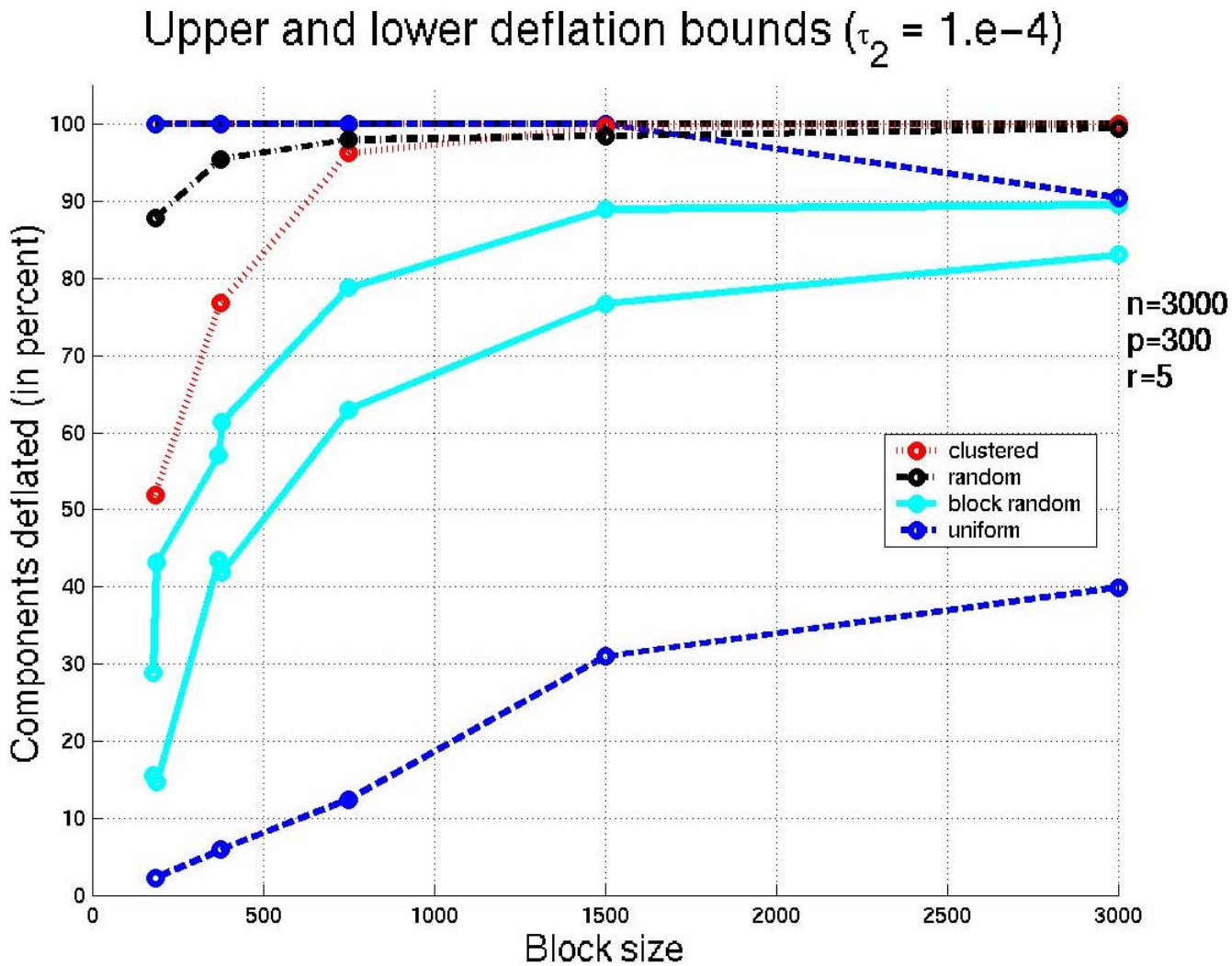
Deflation-Experiments I

- 3 test matrices with prescribed eigenvalue distributions:
  - "clustered": clustered around 0
  - "random": random between -1 and 1
  - "uniform": uniform between -1 and 1
- Additionally, "block random" matrix:
  - random diagonal blocks, off-diagonal blocks from random singular vectors

Deflation-Experiments II



Deflation-Experiments III

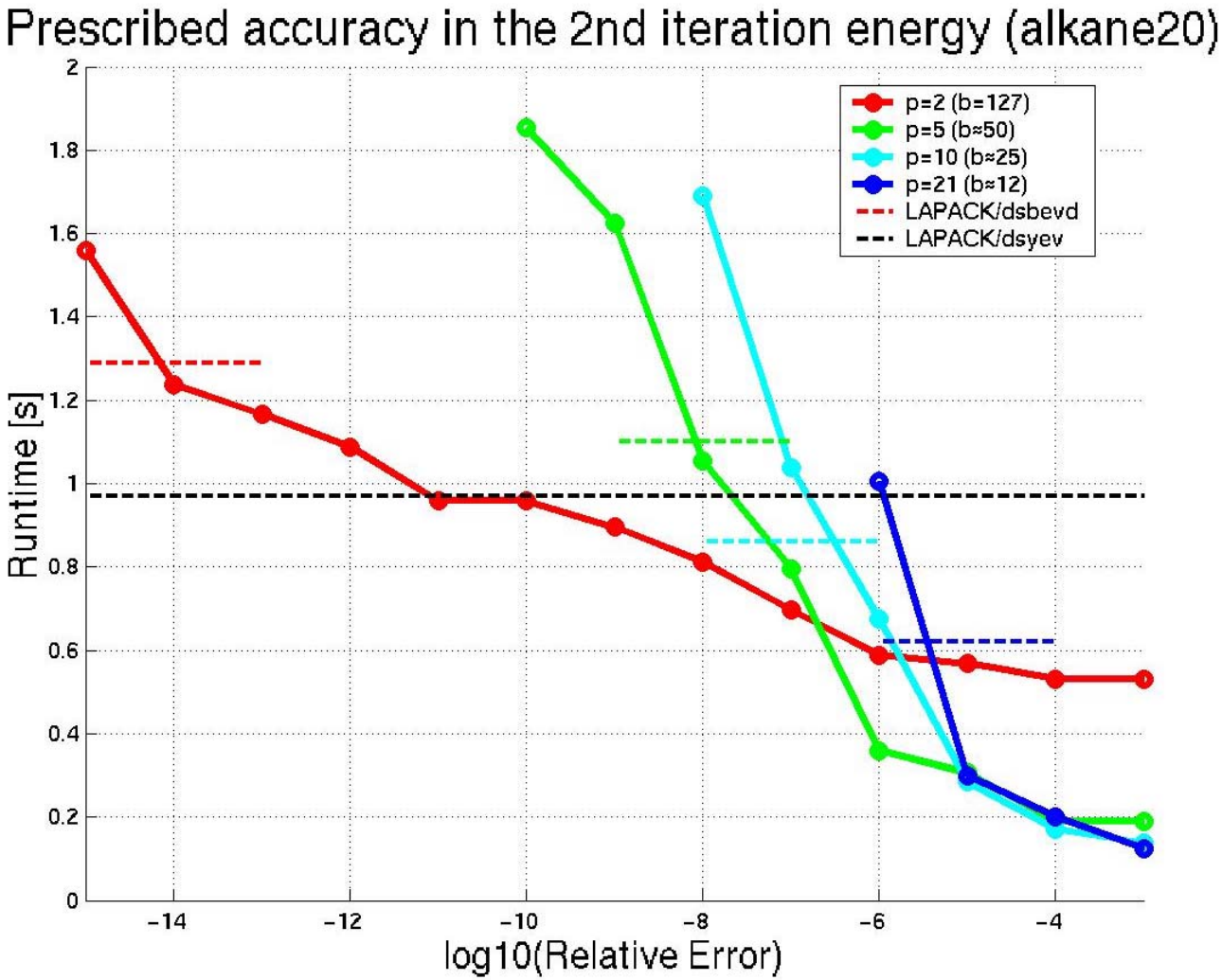


Runtimes -- Comparison with LAPACK

- "block random": n=3000, p=300 (10x10), eigenvectors accumulated, times in [s]

τ_2	r_i=1	r_i=5	r_i=10
LAPACK tolerance	30.2	942.6	2344.6
10^{-10}	23.1	582.6	1429.6
10^{-6}	17.5	229.4	498.8
10^{-2}	11.0	34.8	64.1
dsbevd	1501.7	1529.7	1551.4

Runtimes -- Comparison with LAPACK



QC: SCF Procedure

Compute **S**

Determine **U** s.t. $\mathbf{U^*SU = I}$

Guess $\mathbf{C_0}$

Do i = 0, 1, 2, …

Compute $\mathbf{F(C_i)}$

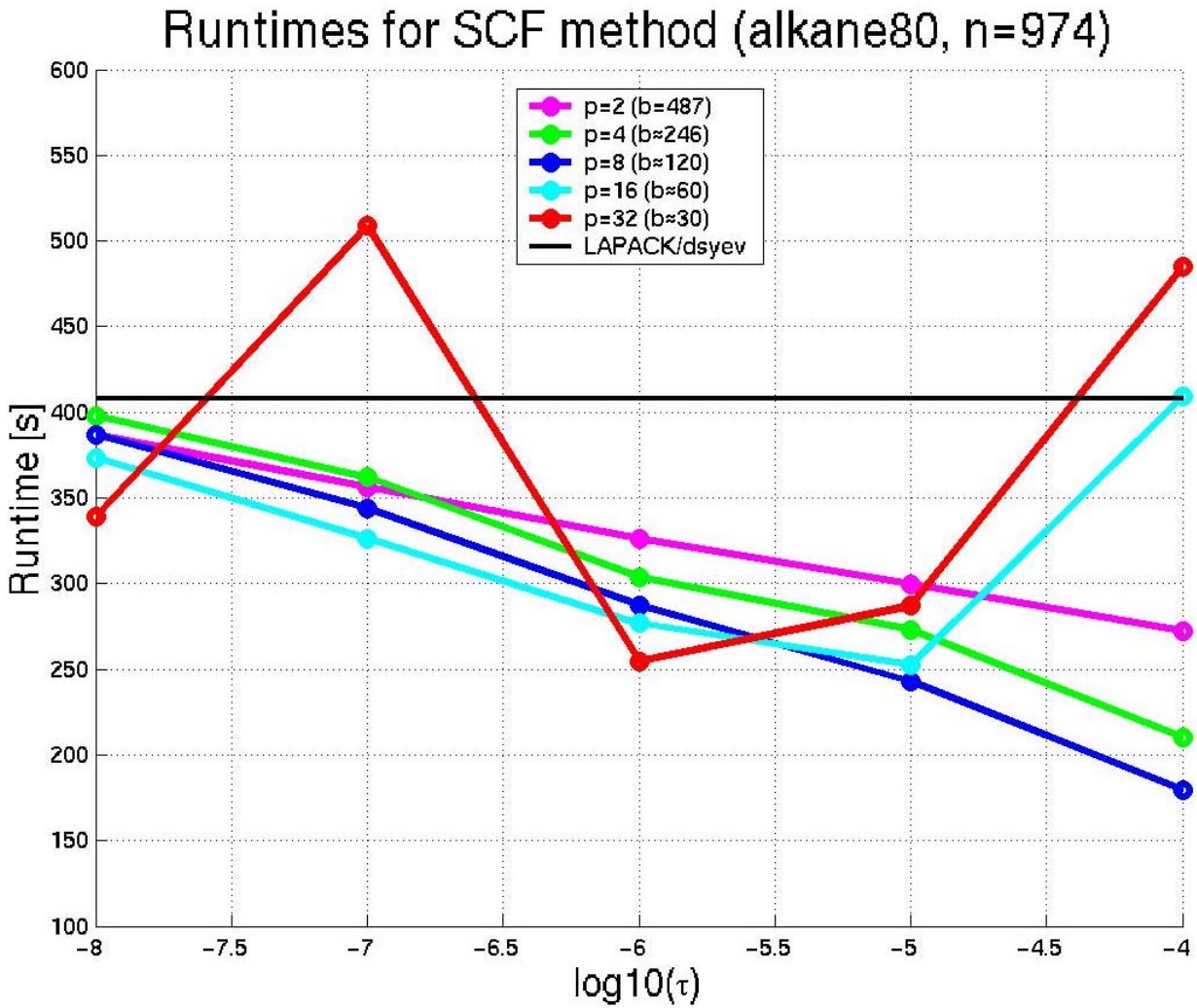
Compute $\mathbf{F'_i = U^*F(C_i)U}$

Solve $\mathbf{F'_iC'_{(i+1)} = C'_{(i+1)}E_{(i+1)}}$ ←

Compute $\mathbf{C_{(i+1)} = UC'_{(i+1)}}$

Check for convergence

Runtimes -- Full SCF Procedure



Experimental Analysis

- Efficient
  - due to good data locality (maps well onto modern memory hierarchies)
  - due to deflation
- Orders of magnitude faster than LAPACK if low accuracy requirements allow for
  - Low rank approximations
  - Large deflation tolerances

Summary and Outlook

Documentation

- Eigenvectors via accumulation
  - Rank-one off-diagonal approximations:
    "An Extension of the Divide-and-Conquer Method for a Class of Symmetric Block-Tridiagonal Eigenproblems", Gansterer, Ward, Muller, 2000. (submitted, also TR UT-CS-00-447)
  - Arbitrary rank off-diagonal approximations:
    "Computing Approximate Eigenpairs of Symmetric Block Tridiagonal Matrices", Gansterer, Ward, Muller, 2001. (submitted, also TR UT-CS-01-463)

Work in Progress/ Future Work

- Alternative eigenvector computation
  - URV decomposition + postprocessing
  - Higher rank modifications, FMM
  - Newton-type approach [Dongarra, Moler, Wilkinson (1983)]
- Higher accuracy
  - Better block-tridiagonal/banded approximation
- Parallelization

Future Work

- Application to QC Problems (CalTech)
  - Utilize information from previous SCF-cycle
  - "Localization"
  - Alternative eigensolvers (Krylov-subspace methods, Jacobi-Davidson,... ?)
  - Methods for *nonlinear* eigenproblems
- Use the framework as a *preconditioner*

More Information

http://www.cs.utk.edu/~cape/