Performance of Block Jacobi-Davidson Eigensolvers

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Numerical method

Eigenvalue problem definition

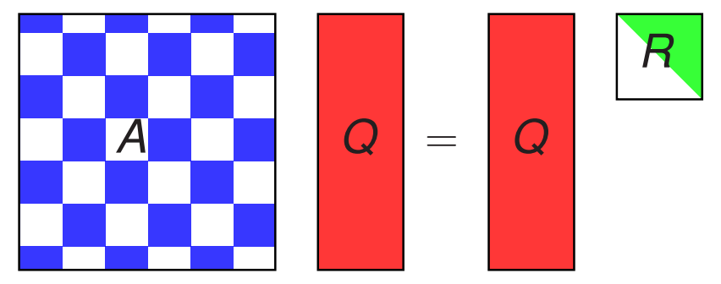
Calculate a small number of extremal eigenpairs (λ_i, v_i) for a sparse, large matrix $A \in \mathbb{C}^{n\times n}$:

$$Av_i = \lambda_i v_i, \qquad i = 1, \dots, l.$$

With an orthonormal basis $Q = (q_1, \dots, q_l)$ for the invariant subspace $\mathcal{V} = \operatorname{span}\{v_1, \dots, v_l\}$ one obtains the more stable block formulation:

$$\begin{cases} AQ - QR &= 0, \\ -\frac{1}{2}Q^*Q + \frac{1}{2}I &= 0. \end{cases}$$

→ Partial Schur decomposition with $r_{i,i} = \lambda_i$:



Block correction equation

In each step of a block Jacobi-Davidson algorithm one calculates correction vectors $\Delta q_1, \dots, \Delta q_l$:

$$\underbrace{(I - \tilde{Q}\tilde{Q}^*)}_{\text{projection onto } Q^\perp} (A - \tilde{\lambda}_i I)(I - \tilde{Q}\tilde{Q}^*)\Delta q_i \approx -(A\tilde{q}_i - \tilde{Q}\tilde{r}_i).$$

Here $(\tilde{Q}, \tilde{R})$ is the current approximation with $\tilde{\lambda}_i = r_{i,i}$ and the column vectors $\tilde{r}_i$ of $\tilde{R}$.

Comparison to the single-vector JDQR

The single-vector JDQR correction equation is

$$(I - \bar{Q}\bar{Q}^*)(A - \tilde{\lambda}I)(I - \bar{Q}\bar{Q}^*)\Delta q \approx -(I - Q_k Q_k{}^*)(A\tilde{q} - \tilde{\lambda}\tilde{q})$$

with converged Schur vectors Q_k and $\bar{Q} = (Q_k \ \tilde{q})$.

→ Both RHS represent deflated residuals.

→ We use a deflation with the complete block $\tilde{Q}$.

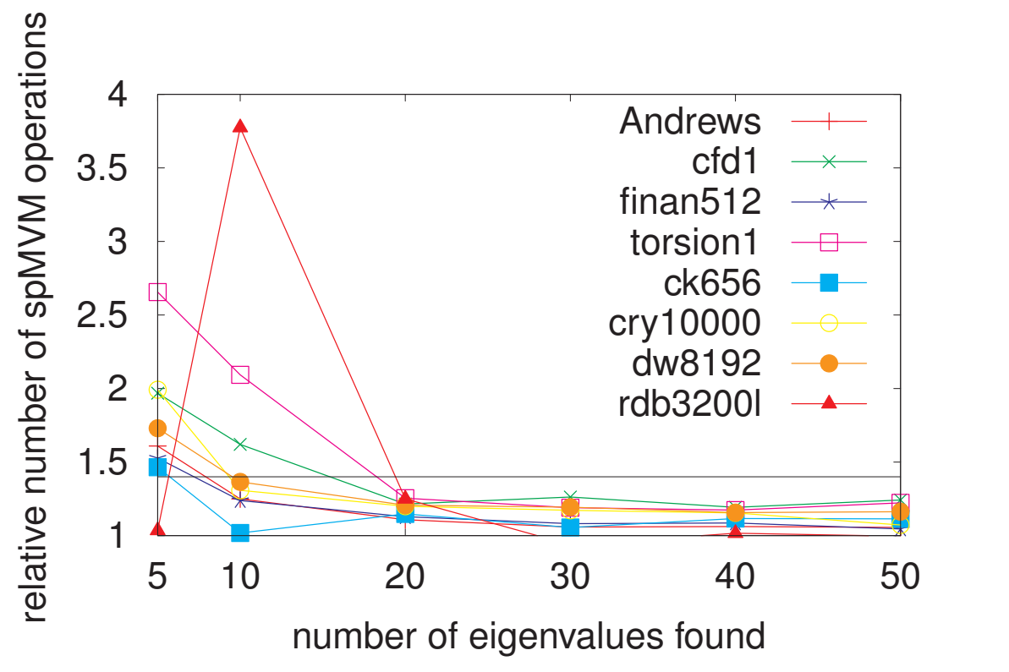
Additional operations due to blocking

- Blocking increases the number of operations (but blocked operations are faster).

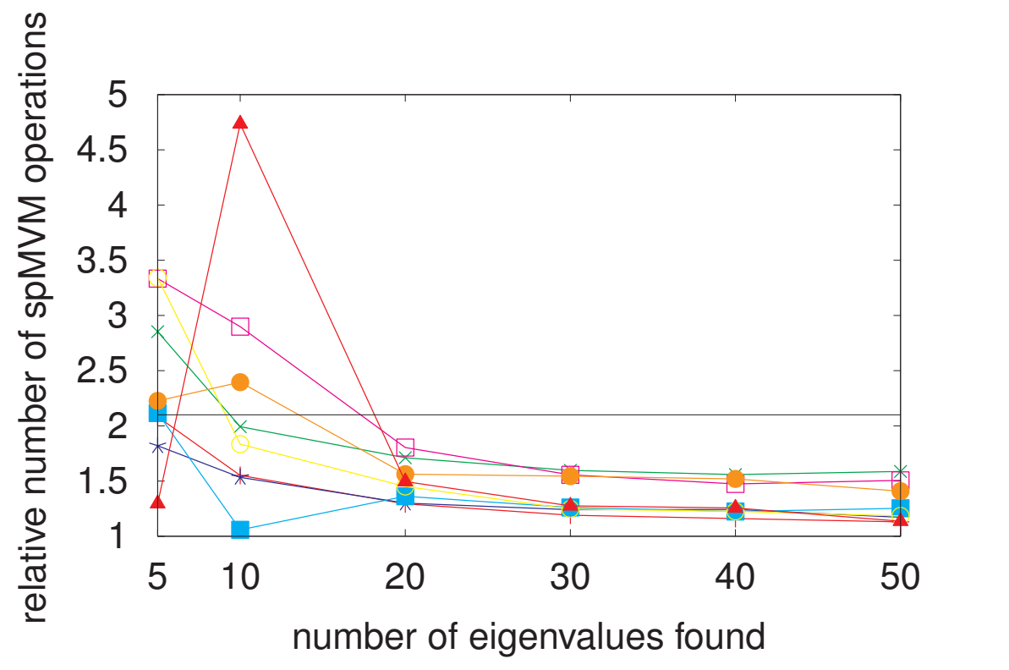
→ Question: How large is the overhead?

- Approach to estimate possible performance gains:
  - Count sparse matrix-vector multiplications (spMVM).
  - Relate results to the performance of block spMVMs.

→ For more than 20 eigenpairs blocking may be beneficial.



(a) Block size 2



(b) Block size 4

Figure: Number of spMVMs of block JDQR compared to single-vector JDQR. The black horizontal line indicates the spMVM block-speedup for a representative matrix (cf. Fig. 4)

Blocked linear solvers

Requirements for blocked iterative solvers

- Concurrently solve l_b systems with different shifts.
- Group together similar operations of different systems.

→ Employ faster block spMVM and block-vector operations.

→ Reduce the number of MPI messages.

- Dynamic queue:
  - Remove converged systems.
  - Enqueue new systems.

Blocked GMRES algorithm

- Standard restarted GMRES method (unpreconditioned)
- Single iteration:

```
1: Apply operator to preceding basis vector
   $(\tilde{v}_{k+1} \leftarrow (I - \tilde{Q}\tilde{Q}^*)(A - \tilde{\lambda}_j)v_k)$,
2: orthogonalize $\tilde{v}_{k+1}$ wrt. all previous basis vectors,
3: perform local operations (Givens rotations, ...).
```

- Basis vectors stored as blocks in a ring buffer (Fig. 2)
- Individual systems can be restarted (when buffer is full).

Blocked MINRES algorithm

- Standard MINRES method (unpreconditioned)
- Very similar to blocked GMRES:
  - Based on Lanczos recurrence instead of modified Gram-Schmidt (for orthogonalization).
  - Store subspace and update result at the end.

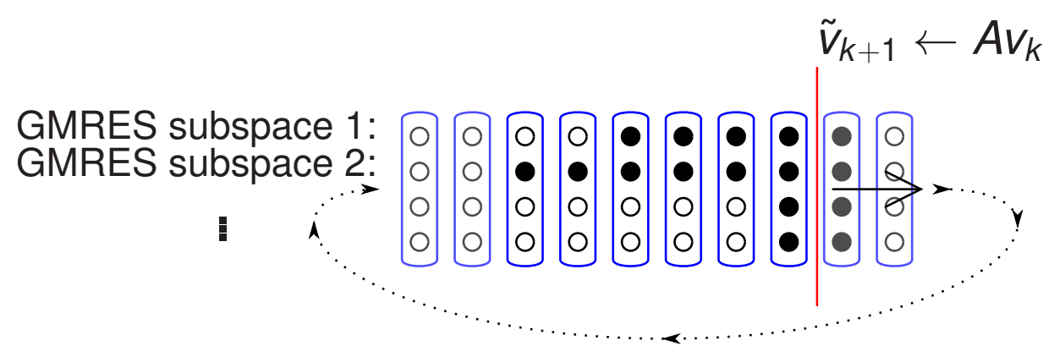


Figure: A partly filled ringbuffer for 4 systems. The data structure allows block operations while using different Krylov subspaces.

Performance engineering of the key operations

Jacobi-Davidson operator

- Required in each inner iteration (iterative solver for the block correction equation)
- Calculate block vector Y for given $X = (x_1, \dots, x_l)$ with

$$y_j \leftarrow (I - QQ^T)(A - \tau_j I)x_j\,.$$

- Shifted sparse matrix–multiple-vector multiplication (spMMVM) can be applied in one step

Sparse matrix–multiple-vector multiplication

- The block vector storage scheme matters (see Fig. 4):

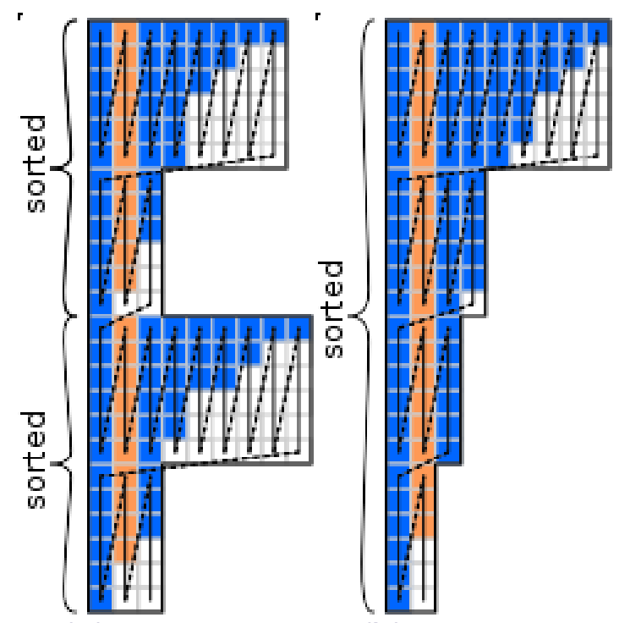
→ Column-major scheme (standard) not beneficial

→ Row-major scheme significantly faster

- Experiments with different sparse matrix formats (CRS vs. SELL-C-σ)
- The Roofline performance model gives helpful insight.

SELL-C-σ format [2]

- parameterized 'sliced ELLPACK'
- competitive on CPU, GPU and MIC alike
- C: chunk size (zero padding)
- σ: sorting scope (to reduce overhead)



(a) SELL-6-12 (b) SELL-6-24

Block vector operations

- Block vectors are dense 'tall skinny' matrices.

→ GEMM operations

- Performance is memory bound due to operands shape (and well predicted by the roofline model).
- Hand-optimized code faster than common BLAS libraries

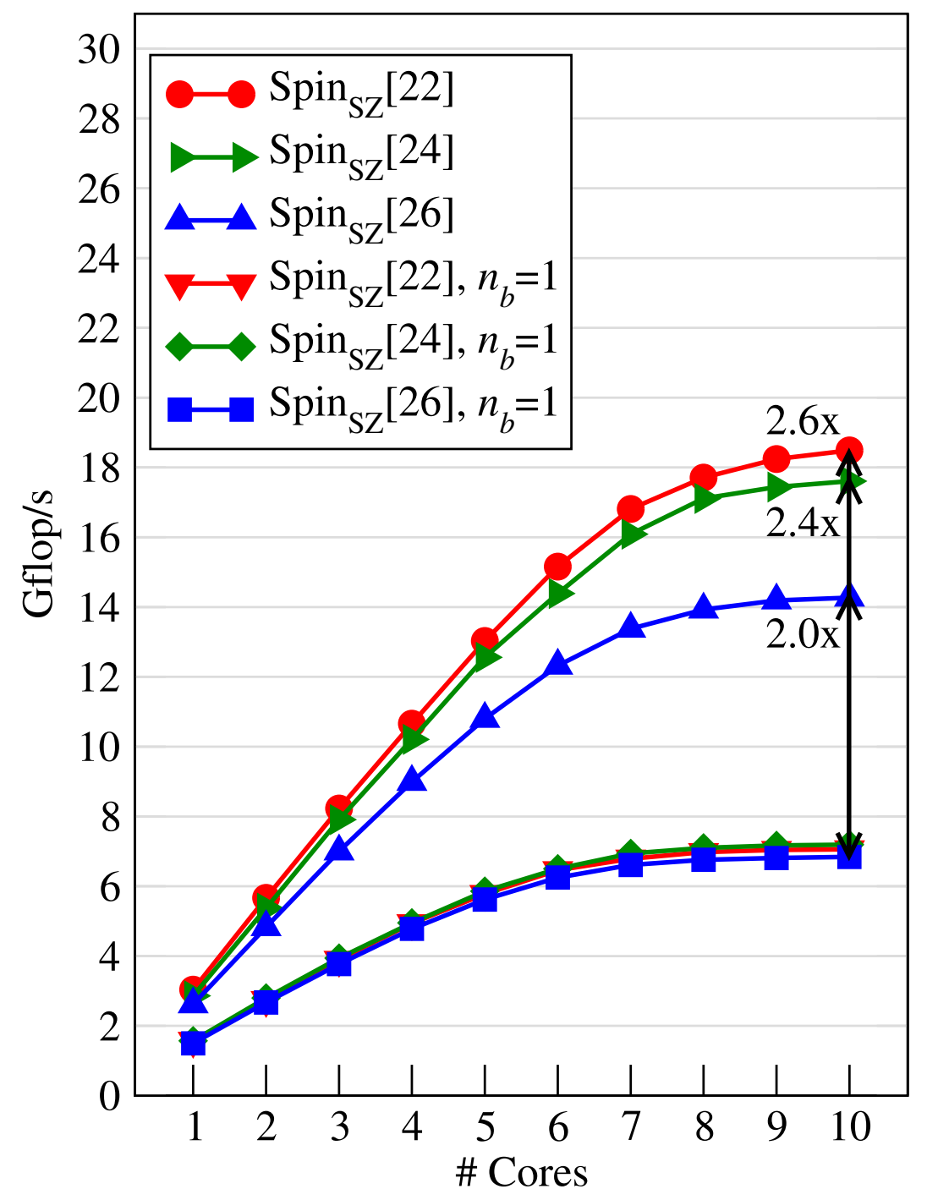


Figure: Intra-socket scaling of spMMVM for spin matrices of different sizes ($\mathrm{Spin}_{SZ}[22] \dots \mathrm{Spin}_{SZ}[26]$)

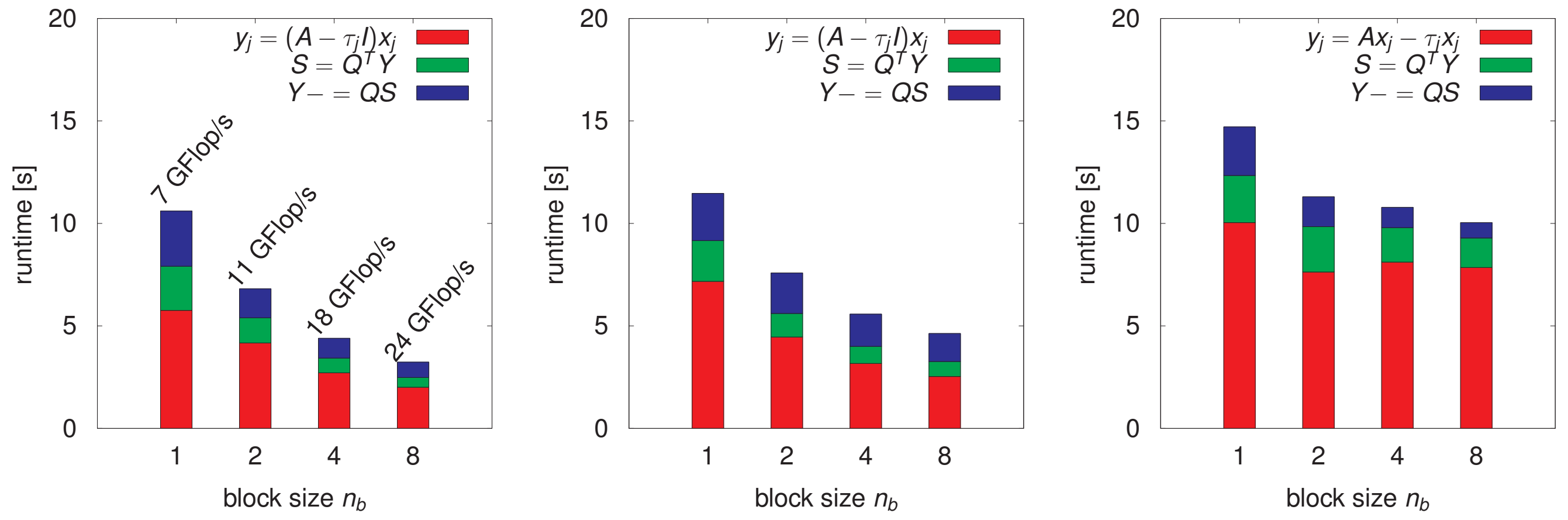


Figure: Single-socket performance of key operations (spMMVM+projections) with the SIMD-friendly SELL-C-σ matrix format [2] from GHOST (left) vs. the standard CRS format (center) and the Epetra CRS format (right). The latter package uses column-major ordering for block vectors and requires an additional copy operation of the entire input vector ('import').

Applications from quantum physics

The $\mathrm{Spin}_{SZ}[L]$ matrices

- Generic benchmark problem from quantum physics
- Chain of L electron spins $^1/_2$, closed to a ring (Fig. 5)
- Computational representation of Hamilton operator in terms of bit patterns & bit swap/flip operations
- Find a few eigenvalues at the left end of the spectrum (lowest energy states)
- Symmetric matrix, can have lots of multiple eigenvalues
- Matrix dimension $\binom{L}{L/2}$ grows exponentially with L

name	number of rows	non-zero count
$\mathrm{Spin}_{SZ}[26]$	$1.0 \cdot 10^7$	$1.5 \cdot 10^8$
$\mathrm{Spin}_{SZ}[28]$	$4.0 \cdot 10^7$	$6.1 \cdot 10^8$
$\mathrm{Spin}_{SZ}[30]$	$1.6 \cdot 10^8$	$2.6 \cdot 10^9$

Table: Dimension of the matrices used in the experiments.

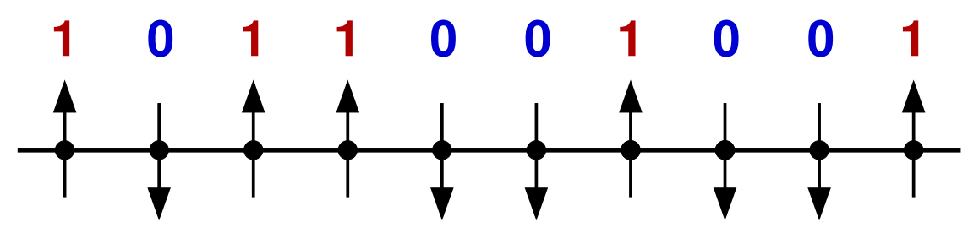


Figure: Chain of 10 electrons with spin up (1) or down (0).

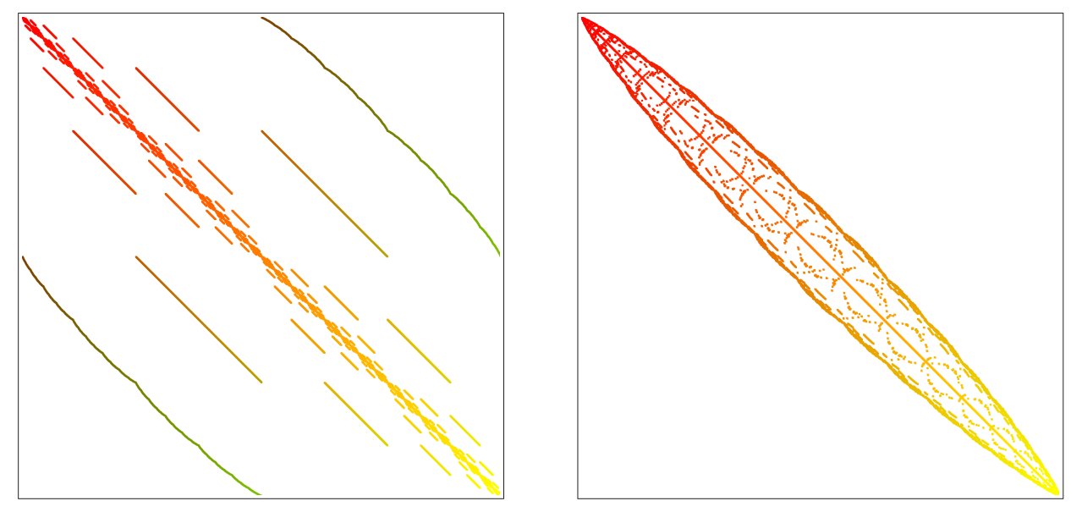


Figure: Typical sparsity structure of the $\mathrm{Spin}_{SZ}[L]$ matrices (here $L = 20$). On the right a bandwidth-reducing preordering was applied.

Block performance in strong scaling experiments

Setup

- Sparse matrices and vectors distributed on a cluster of 1-64 nodes (using MPI)
- Dual socket nodes with 10 cores per socket (using OpenMP parallelization)
- Intel Xeon E5-2660 v2 CPUs ('Ivy bridge') at 2.20 GHz

Results

- Significant speedup of Jacobi-Davidson through blocking in contrast to the conclusion in [1]
- This holds for strong scaling tests on up to 1280 cores.
- Small block sizes (2 or 4) are beneficial.
- Further effects of blocking:
  - Total communication volume increases (spMVMs).
  - Message aggregation may improve the performance.
- See [3] for a detailed discussion.

Future work

- Overlap communication and computation:
  - alleviate increased data traffic due to blocking
- Use accelerator hardware such as GPUs.

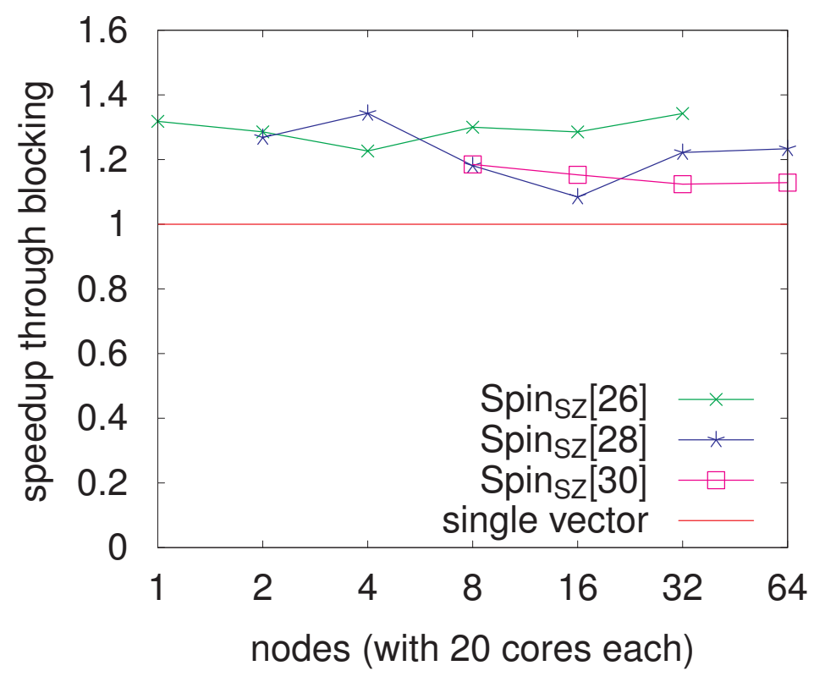
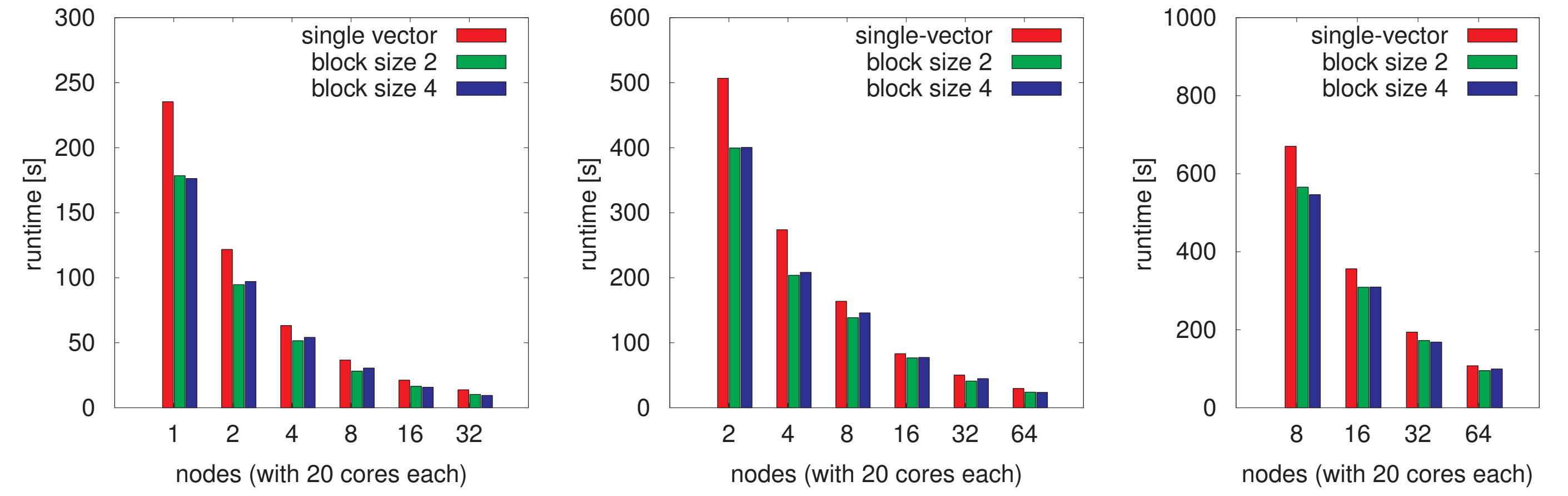


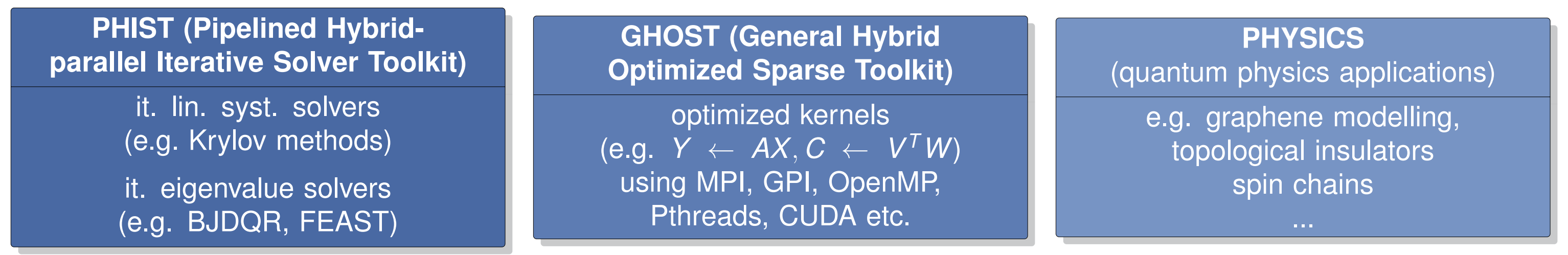
Figure: Relative performance gains with block size 2.



(a) $\mathrm{Spin}_{SZ}[26]$ (b) $\mathrm{Spin}_{SZ}[28]$ (c) $\mathrm{Spin}_{SZ}[30]$

Figure: Strong scaling results for block sizes 2 and 4.

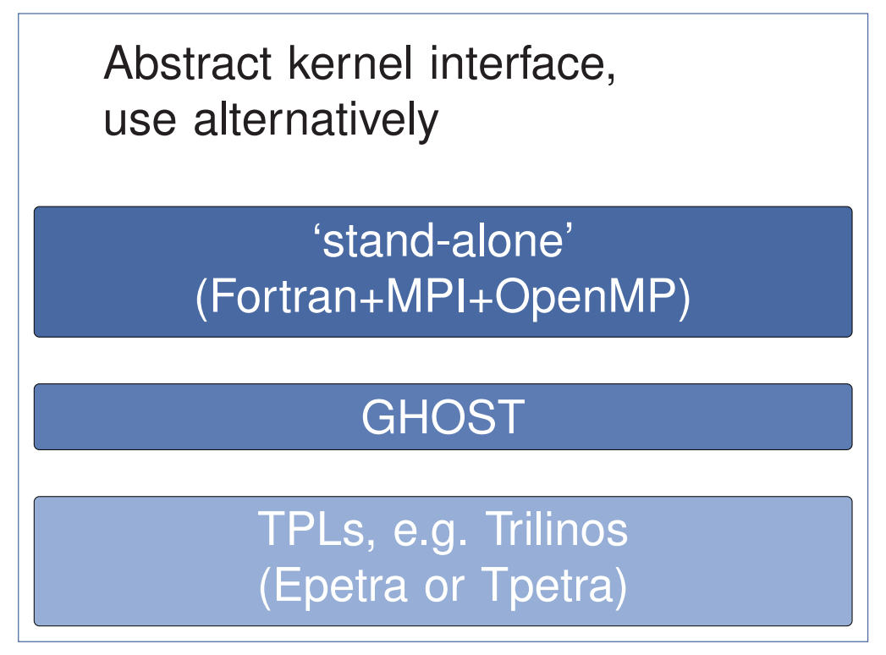
Software



PHIST (Pipelined Hybrid-parallel Iterative Solver Toolkit)
it. lin. syst. solvers
(e.g. Krylov methods)
it. eigenvalue solvers
(e.g. BJDQR, FEAST)

GHOST (General Hybrid Optimized Sparse Toolkit)
optimized kernels
(e.g. $Y \leftarrow AX, C \leftarrow V^T W$)
using MPI, GPI, OpenMP, Pthreads, CUDA etc.

PHYSICS
(quantum physics applications)
e.g. graphene modelling,
topological insulators
spin chains
...



Abstract kernel interface,
use alternatively

'stand-alone'
(Fortran+MPI+OpenMP)

GHOST

TPLs, e.g. Trilinos
(Epetra or Tpetra)

While the software from the ESSEX project has not been publicly released, users interested in early testing are welcome to contact the authors.
Latest news and contact information:

- `http://blogs.fau.de/essex/`
- GHOST: `moritz.kreutzer@fau.de`
- PHIST: `jonas.thies@dlr.de`
- PHYSICS: `alvermann@physik.uni-greifswald.de`
- preprint on the topic available [3]

References

[1] Stathopoulos & McCombs.
Nearly optimal preconditioned methods for Hermitian eigenproblems under limited memory. Part II: Seeking many eigenvalues.
SISC, 29(5), 2007.

[2] Kreutzer *et al.*
A unified sparse matrix data format for modern processors with wide SIMD units.
SISC (accepted) arXiv:1307.6209, 2014.

[3] Röhrig-Zöllner *et al.*
Increasing the performance of the Jacobi-Davidson method by blocking.
SISC (submitted) `http://elib.dlr.de/89980/`, 2014.

ESSEX – Equipping Sparse Solvers for Exascale – funded by the German DFG priority program 1648 '"Software for Exascale Computing"' (SPPEXA) WWW: `http://blogs.fau.de/essex`