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Performance Engineering of the Kernel Polynomial Method on Large-Scale CPU-GPU Systems

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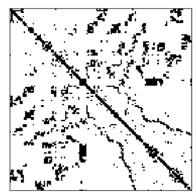
Prologue

What is this about?

The Kernel Polynomial Method (KPM)

Approximate the complete eigenvalue spectrum of a large sparse matrix.

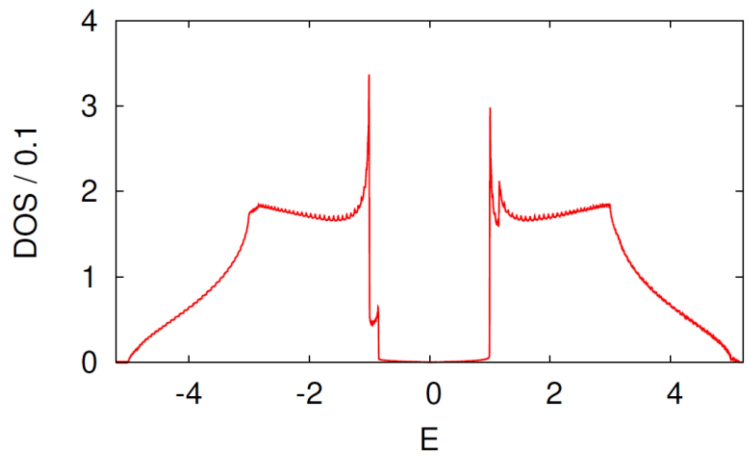
Large, Sparse



$$\boldsymbol{H}\,\boldsymbol{x} = \lambda\,\boldsymbol{x}$$

$$\underbrace{\{\lambda_1, \lambda_2, \dots, \lambda_k, \dots, \lambda_{n-1}, \lambda_n\}}$$

Good approximation to full spectrum
(e.g. Density of States)

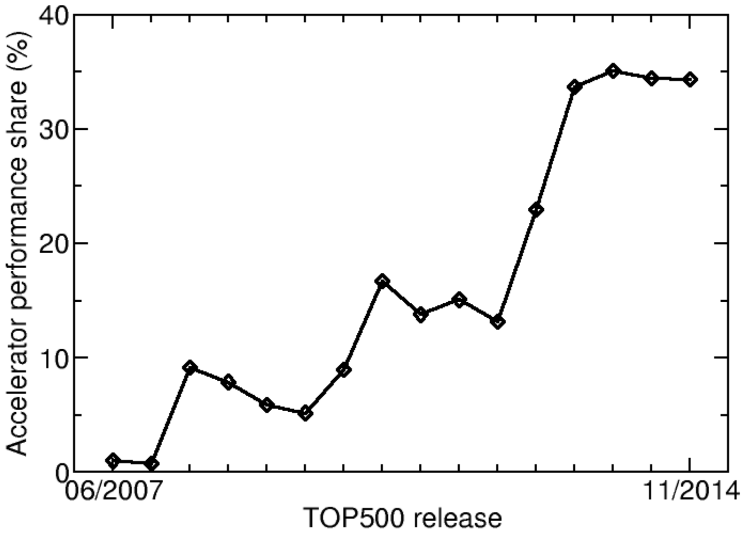


A. Weiße, G. Wellein, A. Alvermann, H. Fehske: **"The kernel polynomial method"**, Rev. Mod. Phys., vol. 78, p. 275, 2006.
E. di Napoli, E. Polizzi, Y. Saad: **"Efficient estimation of eigenvalue counts in an interval"**, Preprint. http://arxiv.org/abs/1308.4275

Why optimize for heterogeneous systems?

One third of TOP500 performance stems from accelerators.

But: Few <u>truly</u> heterogeneous software.
(Using both CPUs and accelerators.)



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The Kernel Polynomial Method

Algorithmic Analysis

The Kernel Polynomial Method

Compute Chebyshev polynomials and moments.

Basic algorithm and algorithmic optimizations:

Exploit knowledge from all software layers!

Building blocks: (Sparse) linear algebra library

for $r = 0$ to $R-1$ **do** — Application: Loop over random initial states
  $|v\rangle \leftarrow |\mathrm{rand}()\rangle$
  Initialization steps and computation of η_0, η_1
  for $m = 1$ to $M/2$ **do** — Algorithm: Loop over moments
    $\mathrm{swap}(|w\rangle, |v\rangle)$
    $|u\rangle \leftarrow H|v\rangle$ ▷ `spmv()` Sparse matrix vector multiply
    $|u\rangle \leftarrow |u\rangle - b|v\rangle$ ▷ `axpy()` Scaled vector addition
    $|w\rangle \leftarrow -|w\rangle$ ▷ `scal()` Vector scale
    $|w\rangle \leftarrow |w\rangle + 2a|u\rangle$ ▷ `axpy()` Scaled vector addition
    $\eta_{2m} \leftarrow \langle v|v\rangle$ ▷ `nrm2()` Vector norm
    $\eta_{2m+1} \leftarrow \langle w|v\rangle$ ▷ `dot()` Dot Product
  end for
end for

The Kernel Polynomial Method

Compute Chebyshev polynomials and moments.

Basic algorithm and algorithmic optimizations:

Exploit knowledge from all software layers!

```
for r = 0 to R−1 do
    |v⟩ ← |rand()⟩
    Initialization steps and computation of η0, η1
    for m = 1 to M/2 do
        swap(|w⟩, |v⟩)
        |u⟩      ← H|v⟩              ▷ spmv()
        |u⟩      ← |u⟩ − b|v⟩        ▷ axpy()
        |w⟩      ← −|w⟩              ▷ scal()
        |w⟩      ← |w⟩ + 2a|u⟩       ▷ axpy()
        η2m      ← ⟨v|v⟩             ▷ nrm2()
        η2m+1    ← ⟨w|v⟩             ▷ dot()
    end for
end for
```

```
for r = 0 to R−1 do
    |v⟩ ← |rand()⟩
    Initialization steps and computation of η0, η1
    for m = 1 to M/2 do
        swap(|w⟩, |v⟩)
        |w⟩ = 2a(H − b𝟙)|v⟩ − |w⟩ &
            η2m   = ⟨v|v⟩ &
            η2m+1 = ⟨w|v⟩            ▷ aug_spmv()
end for
```

Augmented Sparse Matrix Vector Multiply

The Kernel Polynomial Method

Compute Chebyshev polynomials and moments.

Basic algorithm and algorithmic optimizations:

Exploit knowledge from all software layers!

for $r = 0$ to $R-1$ **do**
  $|v\rangle \leftarrow |\text{rand}()\rangle$
  Initialization steps and computation of η_0, η_1
  for $m = 1$ to $M/2$ **do**
    $\text{swap}(|w\rangle, |v\rangle)$
    $|u\rangle \leftarrow H|v\rangle$ ▷ `spmv()`
    $|u\rangle \leftarrow |u\rangle - b|v\rangle$ ▷ `axpy()`
    $|w\rangle \leftarrow -|w\rangle$ ▷ `scal()`
    $|w\rangle \leftarrow |w\rangle + 2a|u\rangle$ ▷ `axpy()`
    $\eta_{2m} \leftarrow \langle v|v\rangle$ ▷ `nrm2()`
    $\eta_{2m+1} \leftarrow \langle w|v\rangle$ ▷ `dot()`
  end for
end for

for $r = 0$ to $R-1$ **do**
  $|v\rangle \leftarrow |\text{rand}()\rangle$
  Initialization steps and computation of η_0, η_1
  for $m = 1$ to $M/2$ **do**
    $\text{swap}(|w\rangle, |v\rangle)$
    $|w\rangle = 2a(H - b\mathbb{1})|v\rangle - |w\rangle$ &
    $\eta_{2m} = \langle v|v\rangle$ &
    $\eta_{2m+1} = \langle w|v\rangle$ ▷ `aug_spmv()`
  end for

$|V\rangle := |v\rangle_{0..R-1}$ ▷ Assemble vector blocks
$|W\rangle := |w\rangle_{0..R-1}$
$|V\rangle \leftarrow |\text{rand}()\rangle$
Initialization steps and computation of μ_0, μ_1
for $m = 1$ to $M/2$ **do**
  $\text{swap}(|W\rangle, |V\rangle)$
  $|W\rangle = 2a(H - b\mathbb{1})|V\rangle - |W\rangle$ &
  $\eta_{2m}[:] = \langle V|V\rangle$ &
  $\eta_{2m+1}[:] = \langle W|V\rangle$ ▷ `aug_spmmv()`
end for

Augmented Sparse Matrix Multiple Vector Multiply

Analysis of the Algorithmic Optimization

- **Minimum code balance of vanilla algorithm:**
  complex double precision values, 32-bit indices, 13 non-zeros per row, application: topological insulators

  $B_{vanilla} = 3.39\ Bytes/Flop$ (B = inverse computational intensity)

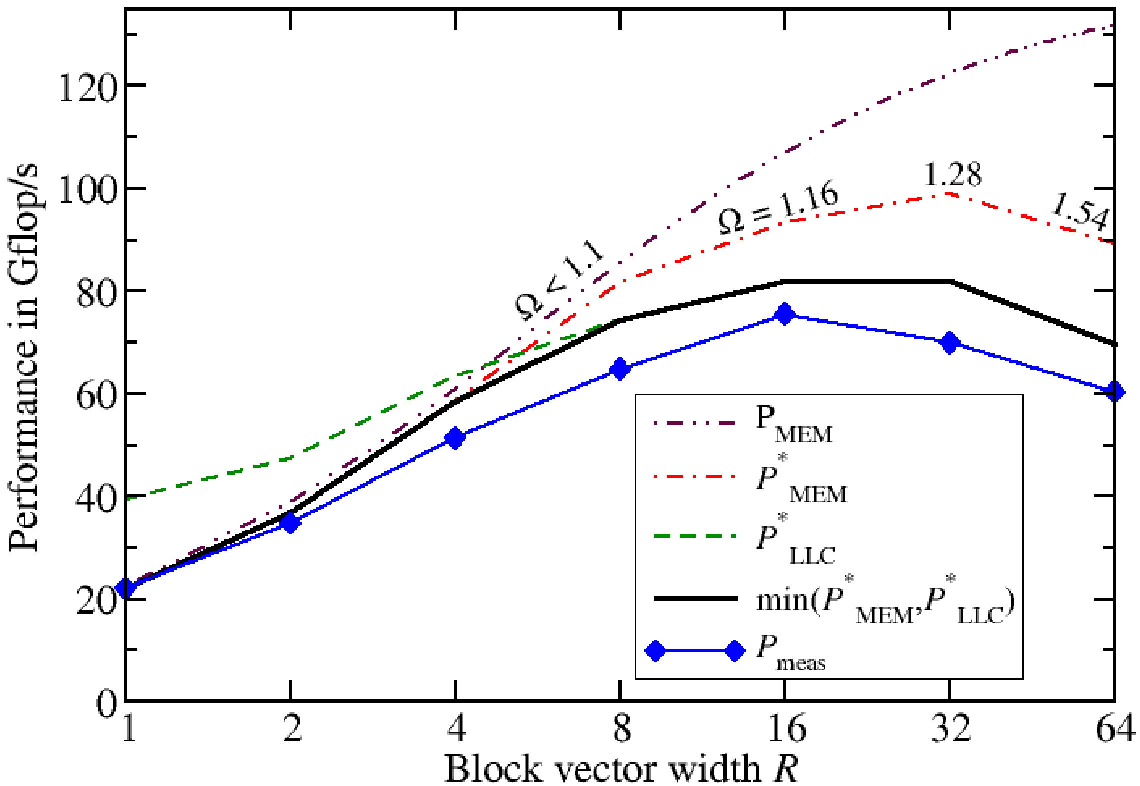
- **Identified bottleneck: Memory bandwidth**
  ➔ Decrease memory transfers to alleviate bottleneck

- **Algorithmic optimizations reduce code balance:**
  $B_{aug\_spmv} = 2.23\ B/F$ kernel fusion
  $B_{aug\_spmmv}(R) = 1.88/R + 0.35\ B/F$ put *R* vectors in block

Consequences of Algorithmic Optimization

- **Mitigation of the relevant bottleneck**
  ➔ Expected speedup ☺
- **Other bottlenecks become relevant**
  ➔ Achieved speedup may not be $B_{vanilla}/B_{aug\_spmmv}$ 😐
- **Block vectors are best stored interleaved**
  ➔ May impose larger changes to the codebase ☹
- `aug_spmmv()` **no part of standard libraries**
  ➔ Implementation by hand is necessary ☹

CPU roofline performance model



$P = \frac{b}{B}$ **Gflop/s**

→ Performance limit for bandwidth-bound code

b = max. bandwidth = 50 GB/s
B = code balance

$\Omega = \frac{\textit{Actual data transfers}}{\textit{Minimum data transfers}}$

Intel Xeon E5-2660v2 "Ivy Bridge"

S. Williams, A. Waterman, D. Patterson: **"Roofline: An insightful visual performance model for multicore architectures"**, *Commun. ACM*, vol. 52, p. 65, 2009.

Implementation

How to harness a heterogeneous machine in an efficient way?

Implementation

Algorithmic optimizations lead to a *potential* speedup.

➔ We "merely" need an efficient implementation!

Data or task parallelism?

- **MAGMA: task parallelism between devices**
  ➔ Kernel fusion ⚡ Task parallelism

➔ Data-parallel approach suits our needs

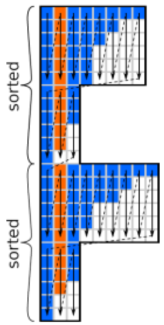
Implementation

Data-parallel heterogeneous work distribution

- Static work-distribution by matrix rows/entries
- Device workload ←→ device performance

SELL-C-σ sparse matrix storage format

- Unified format for all relevant devices
- Currently no runtime-exchange of matrix data (dynamic load balancing, future work)

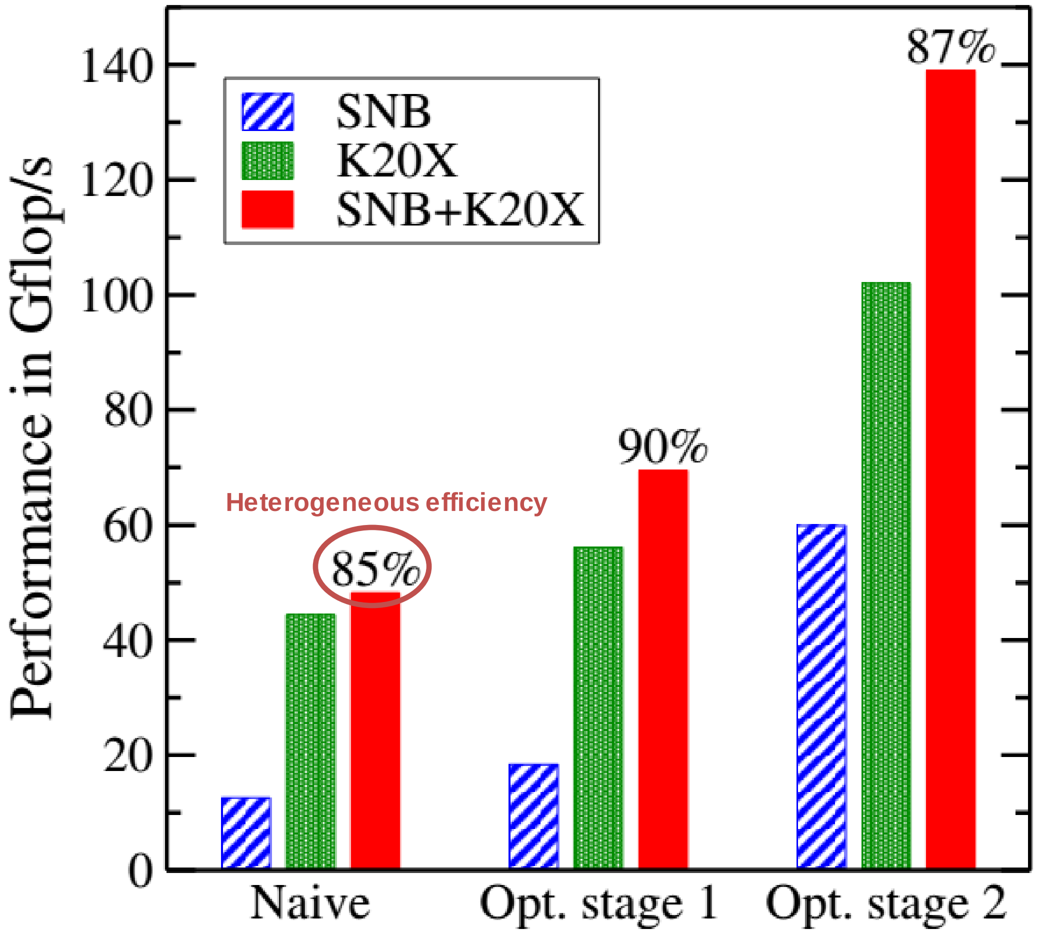


M. Kreutzer, G. Hager, G. Wellein, H. Fehske, A. R. Bishop, **"A unified sparse matrix data format for efficient general sparse matrix-vector multiplication on modern processors with wide SIMD units"**, *SIAM J. Sci. Comput.*, vol. 36, p. C401, 2014

Performance results

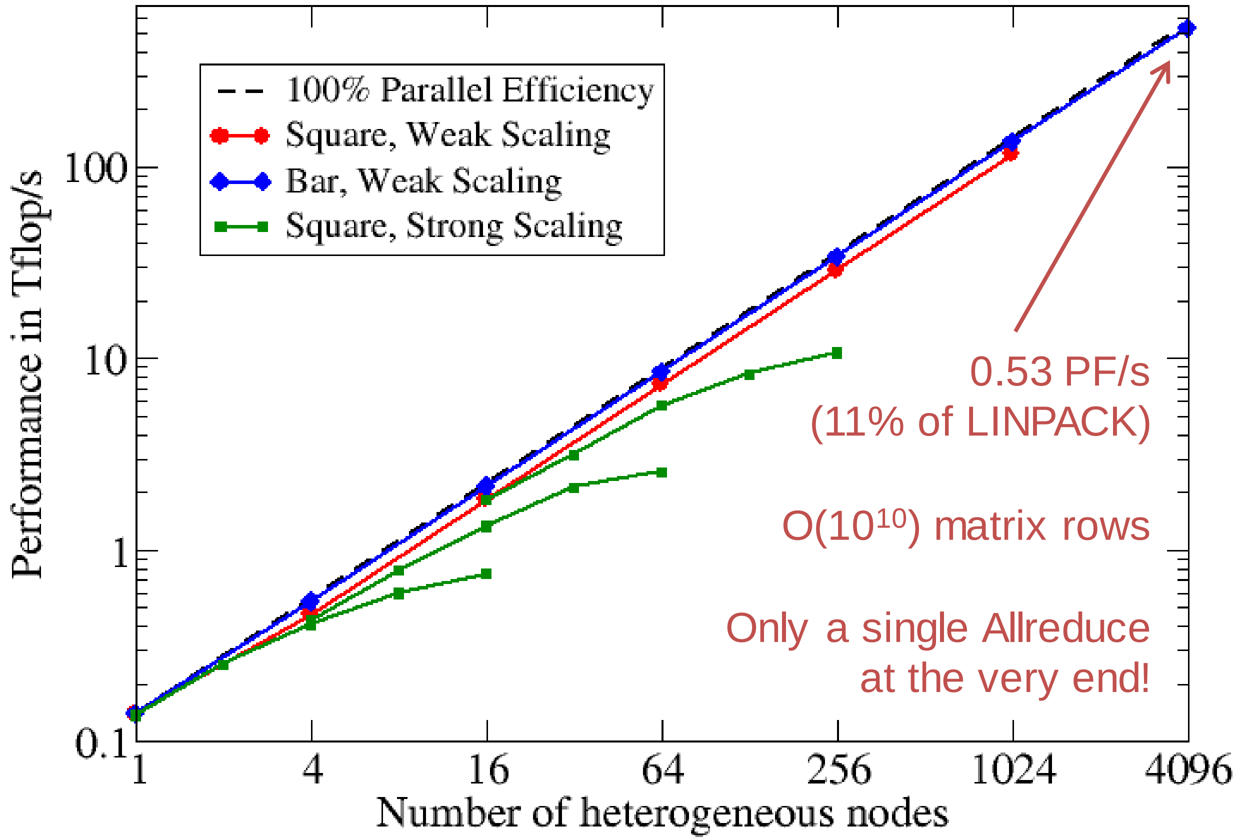
Does all this really pay off?

Single-node Heterogeneous Performance



SNB: Intel Xeon E5-2670 “Sandy Bridge“, K20X: Nvidia Tesla K20X, Complex double precision data (topological insulator)

Large-scale Heterogeneous Performance



CRAY XC30 – Piz Daint*

- 5272 nodes, each w/
  - 1 octacore Intel Sandy Bridge
  - 1 Nvidia Kepler K20x
- Peak: 7.8 Pflop/s
- LINPACK: 6.3 Pflop/s
- Largest system in Europe

*Thanks to CSCS/O. Schenk/T. Schulthess for granting access and compute time

M. Kreutzer, A.Pieper, G.Hager, G. Wellein, A. Alvermann, H. Fehske, **"Performance Engineering of the Kernel Polynomial Method on Large-Scale CPU-GPU Systems"**, *Parallel and Distributed Processing Symposium (IPDPS), 2015 IEEE International*, p. 417-426, 2015

Epilogue

Try it out! (If you want…)

Download our building block library and KPM application: `http://tiny.cc/ghost`

General, Hybrid, and Optimized Sparse Toolkit

- **MPI + OpenMP + SIMD + CUDA**
- **Transparent data-parallel heterogeneous execution**
- **Affinity-aware task parallelism (checkpointing, comm. hiding, etc.)**
- **Support for block vectors**
  - Automatic code generation for common block vector sizes
  - Hand-implemented tall skinny dense matrix kernels
- **Fused kernels (arbitrarily "augmented SpMMV")**
- **SELL-C-σ heterogeneous sparse matrix format**
- **Various sparse eigensolvers implemented and downloadable**

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