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Performance Engineering for Algorithmic Building Blocks in the GHOST Library

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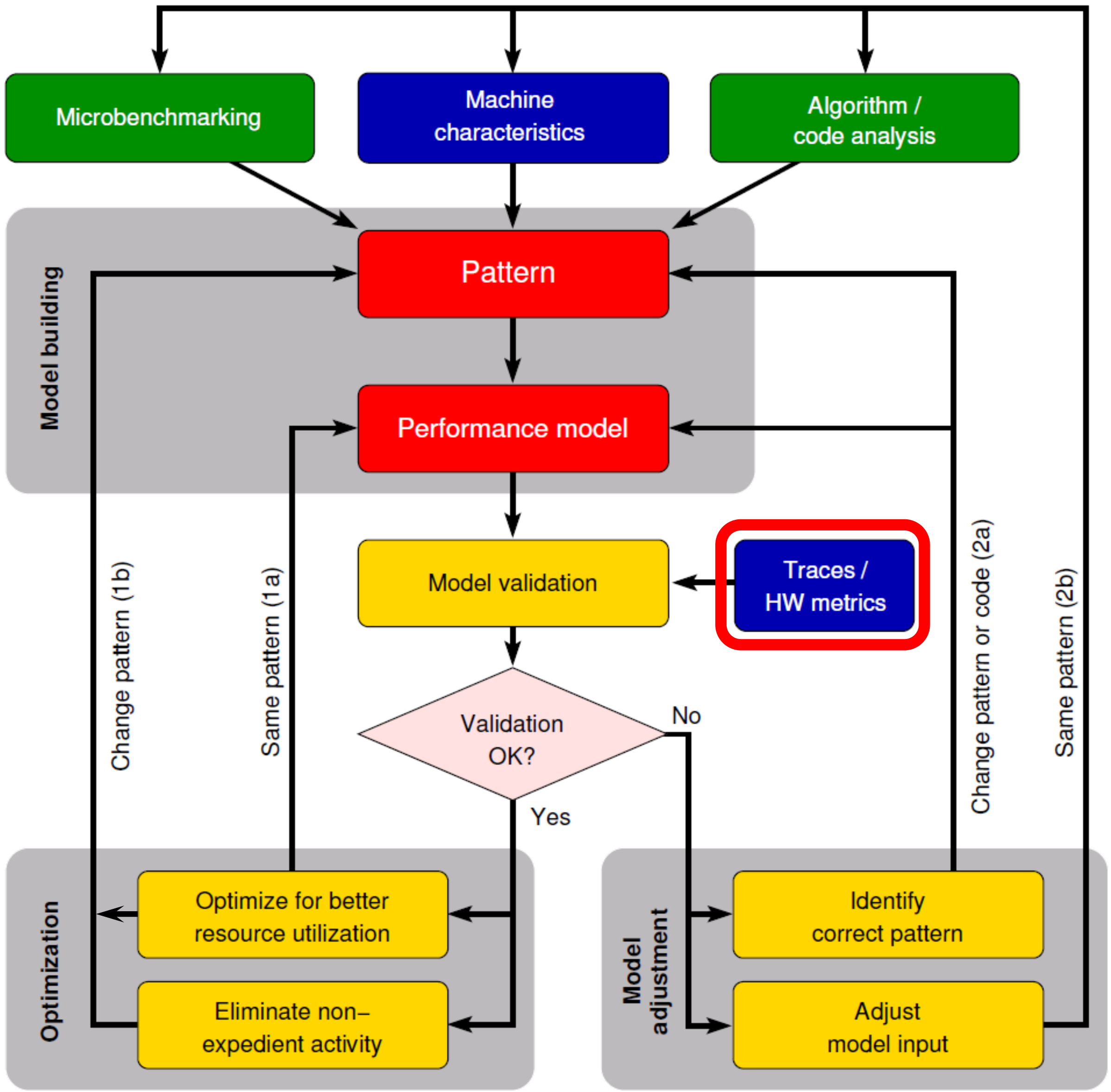
Outline

Performance Engineering (PE)

The GHOST library

Work planned for ESSEX-II

The whole PE process at a glance



Example: KPM

Kernel Polynomial Method

- Compute spectral properties of quantum system (Hamilton operator)
- Approximation of full spectrum
- Naïve implementation: SpMVM + several BLAS-1 kernels

for $r = 0$ to $R-1$ **do** — Application: Loop over random initial states
  $|v\rangle \leftarrow |\text{rand}()\rangle$
  Initialization steps and computation of η_0, η_1
  for $m = 1$ to $M/2$ **do** — Algorithm: Loop over moments
    $\text{swap}(|w\rangle, |v\rangle)$
    $|u\rangle \leftarrow H|v\rangle$ ▷ 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

Building blocks: (Sparse) linear algebra library

Dot Product

- 1 **do**
$\rangle$
steps and computation of η_0, η_1
$M/2$ **do**
$, |v\rangle)$
$(H - b\mathbb{1})|v\rangle - |w\rangle$ &
$= \langle v|v\rangle$ &
$= \langle w|v\rangle$ ▷ aug_spmv()
$[:] = \langle w|v\rangle$ ▷ aug_spmv()

Augmented Sparse Matrix Vector Multiply

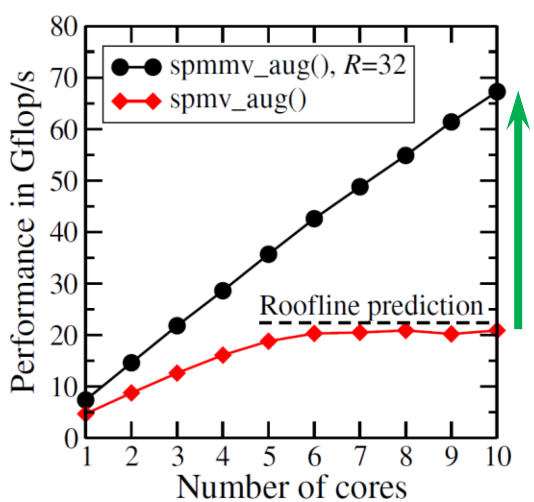
Augmented Sparse Matrix Multiple Vector Multiply

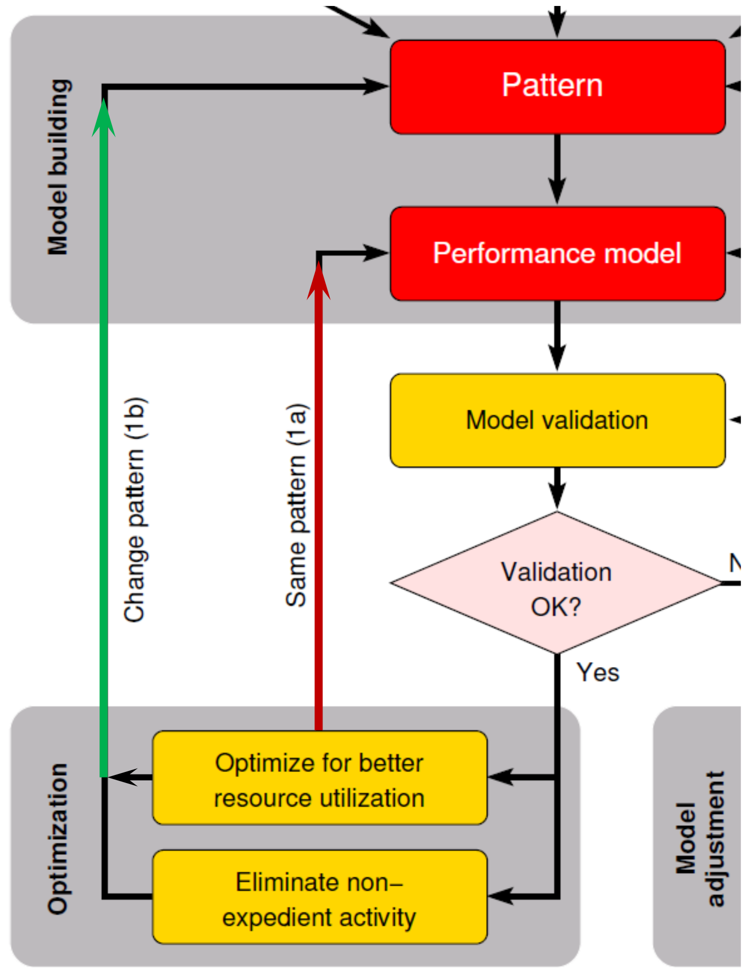
Step 1: naïve → augmented (fused) kernel

- Naïve kernel is clearly memory bound
- Better resource utilization
- B_C = 3.39 B/F → 2.23 B/F
- Still memory bound → same pattern

Step 2: augmented → blocked

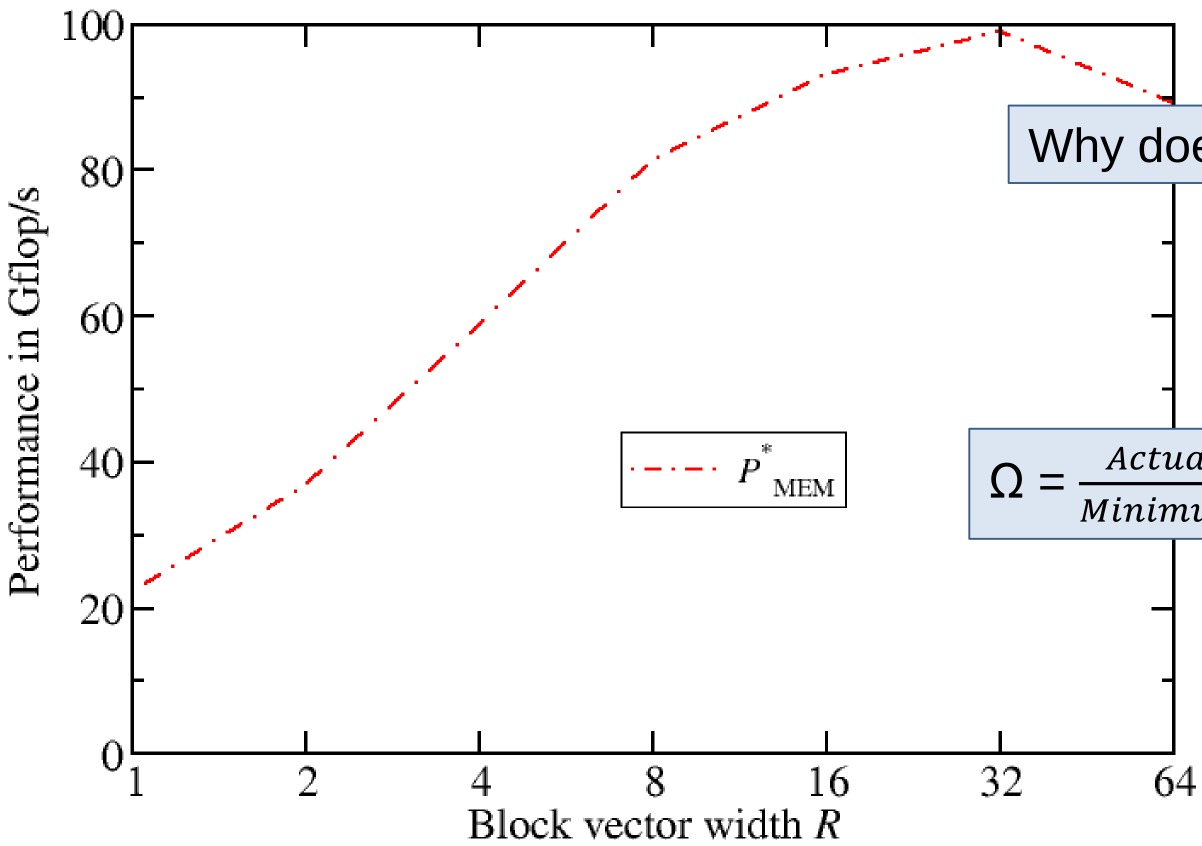
- Augmented kernel is memory bound
- R = # of random vectors
- B_C = 2.23 B/F → (1.88/R + 0.35) B/F
- Decouples from main memory BW





→ **Performance portability** becomes well defined!

What about the decoupled model?



Why does it decrease?

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

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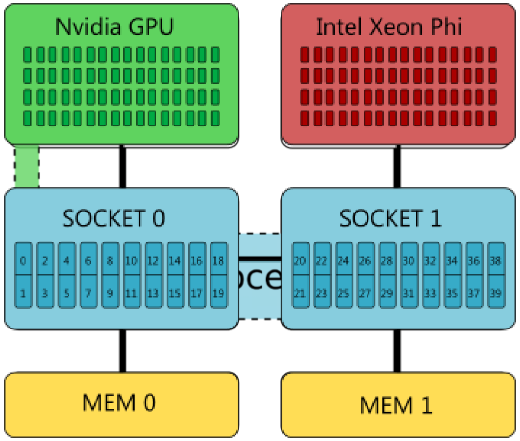
The GHOST library

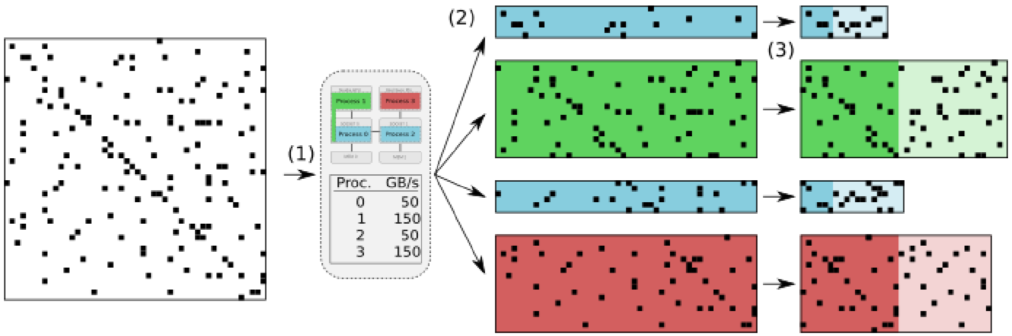
General Hybrid Optimized Sparse Toolkit

M. Kreutzer et al.: GHOST: Building blocks for high performance sparse linear algebra on heterogeneous systems.
Preprint arXiv:1507.08101

GHOST design guidelines

- Strictly support the requirements of the project
- Enable fully heterogeneous operation
- Limit automation
- Do not force dynamic tasking
- Do not force C++ or an entirely new language
- Stick to the well-known “MPI+X” paradigm
- Support data parallelism via MPI+X
- Support functional parallelism via tasking
- Allow for strict thread/process-core affinity





Task parallelism: Asynchronous checkpointing with GHOST tasks

Parent task

```
ghost_task_create( ckpt_task_ptr,&
     CP_func, CP_obj,…)

update_CP(CP_obj);
```

// async. copy of CP is updated

```
ghost_task_wait(ckpt_task_ptr);

ghost_task_enqueue(ckpt_task_ptr);
```

iterative

CP_obj:

- **void*** to object of **ckpt_t** type
- **ckpt_t** class is defined by programmer
- checkpoint object contains the asynchronous copy of the checkpoint

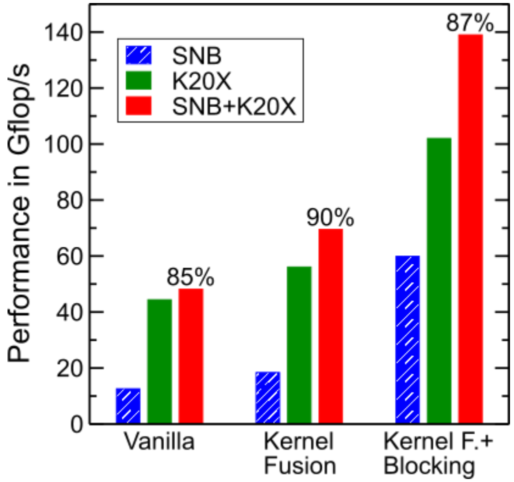
Checkpoint task

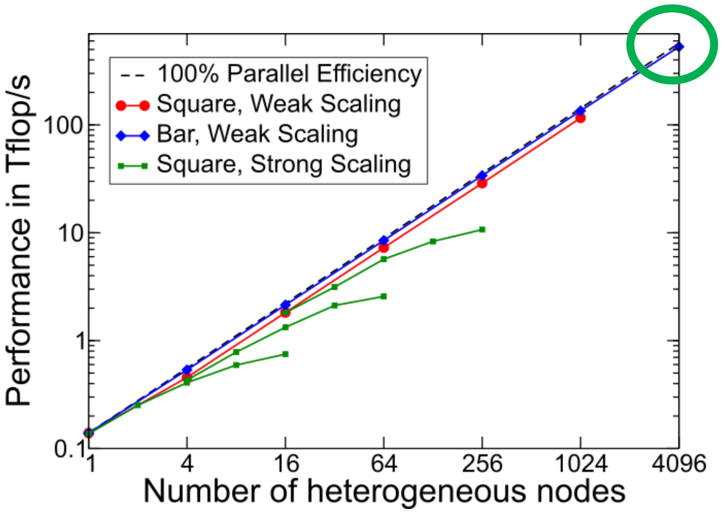
CP_func()

// This function takes an updated copy of **CP_obj** as argument and writes to PFS

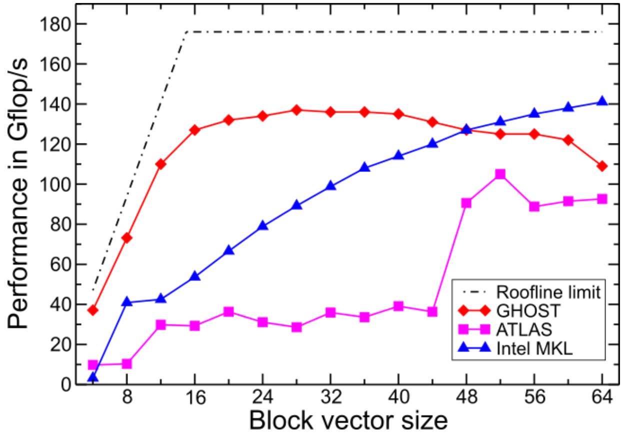
Heterogeneous performance?

0.5 Pflop/s





The need for hand-engineered kernels



Block vector times small matrix performance of GHOST and existing BLAS libraries (*tall skinny ZGEMM*)

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SELL-C-σ

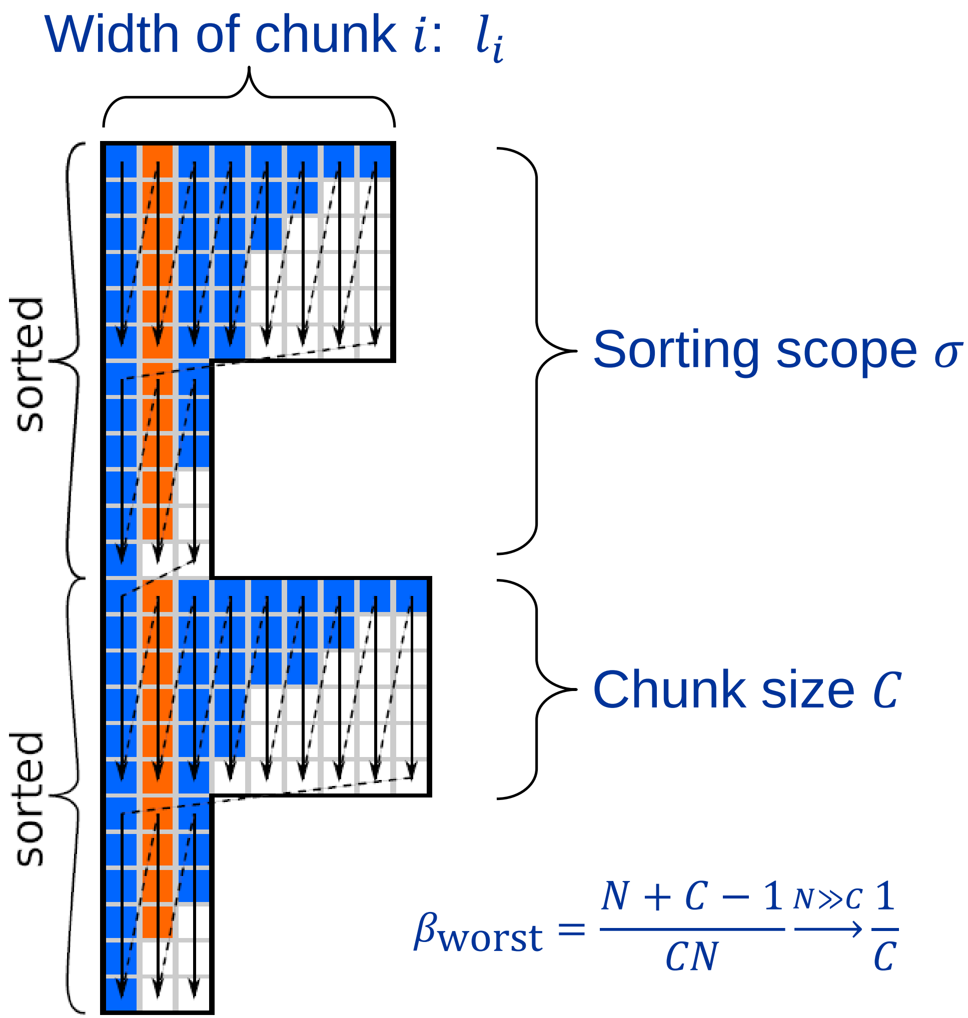
Performance portability for SpMVM

Constructing SELL-C-σ

1. Pick chunk size C (guided by SIMD/T widths)
2. Pick sorting scope σ
3. Sort rows by length within each sorting scope
4. Pad chunks with zeros to make them rectangular
5. Store matrix data in "chunk column major order"

6. "Chunk occupancy": fraction of "useful" matrix entries

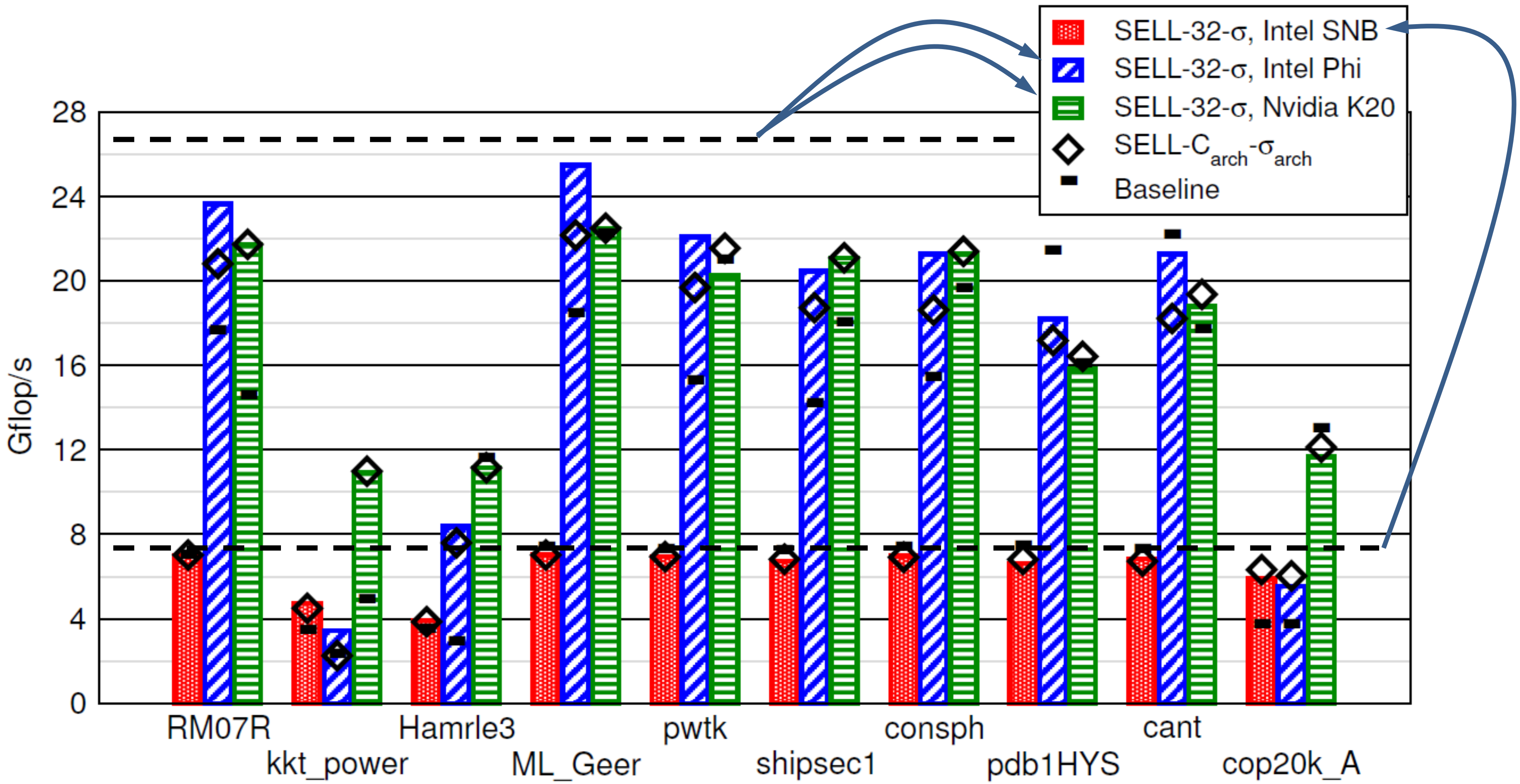
$$\beta = \frac{N_{nz}}{\sum_{i=0}^{N_c} C \cdot l_i}$$



$$\beta_{\text{worst}} = \frac{N + C - 1}{CN} \xrightarrow{N \gg C} \frac{1}{C}$$

SELL-6-12
β=0.66

What is performance portability?



ESSEX-II and GHOST

1. **Building blocks development**
    - Improved support for mixed precision kernels
    - Fast point-to-point sync on many-core
    - High-precision reductions
    - (Row-major storage TSQR)
    - Full support for heterogeneous hardware (CPU, GPGPU, Phi)
2. **Optimized sparse matrix data structures**
    - Identify promising candidates (ACSR, CSX)
    - Exploiting matrix structure: symmetry, sub-structures
3. **Holistic power and performance engineering**
    - Comprehensive instrumentation of GHOST library functions
    - **ECM performance modeling of SpMMVM and others**
    - **Energy modeling of building blocks**
    - Performance modeling beyond the node
4. **Comprehensive documentation**

Example: performance impact of the Kahan-augmented dot product

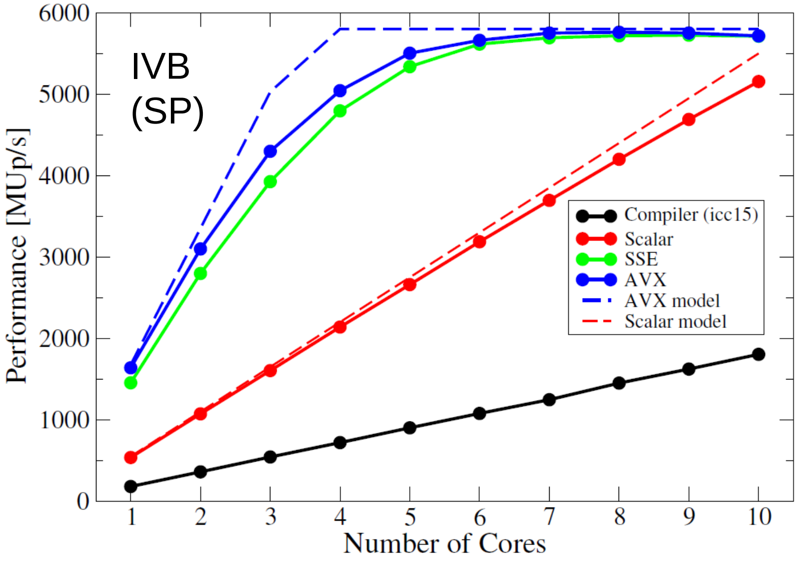
```
float sum = 0.0;
  for (int i=0; i<N; i++) {
  sum = sum + a[i] * b[i]
}
```

1 ADD, 1 MULT

```
float sum = 0.0, c = 0.0;
for (int i=0; i<N; ++i) {
  float prod = a[i]*b[i];
  float y = prod-c;
  float t = sum+y;
  c = (t-sum)-y;
  sum = t;
}
```

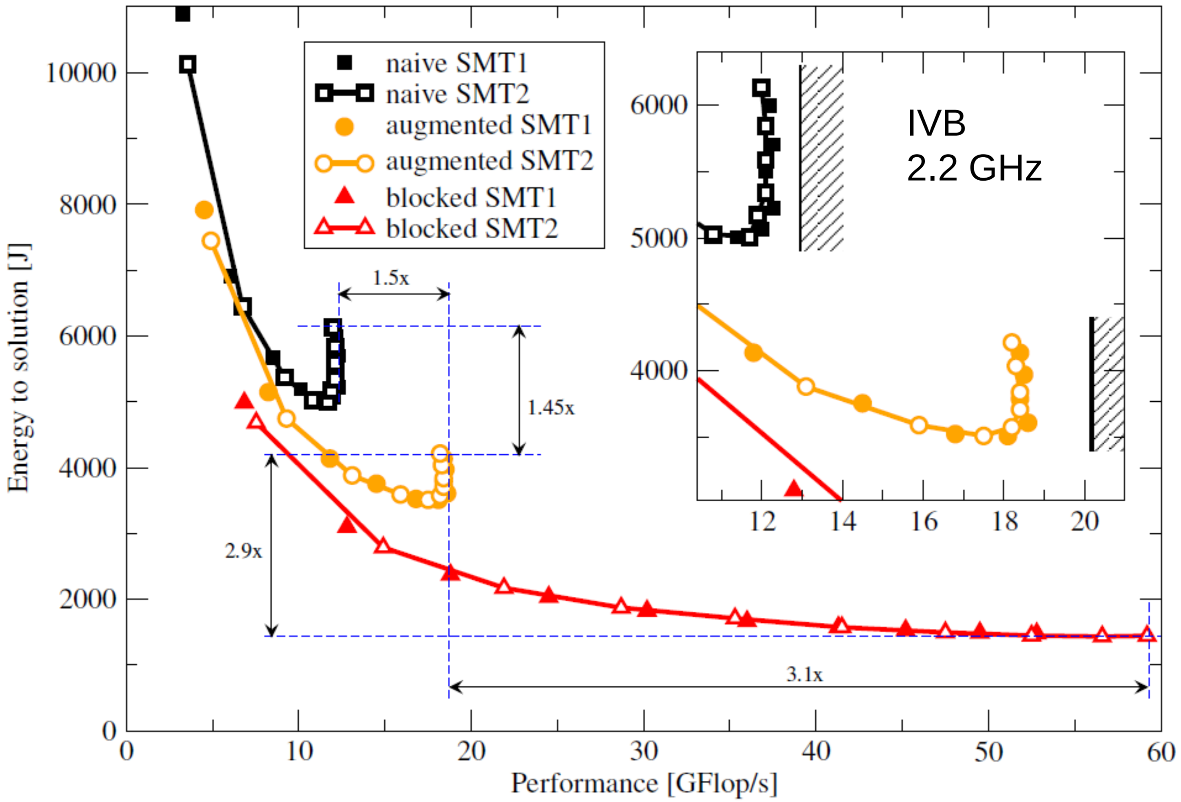
4 ADD, 1 MULT

- No impact of Kahan if *any* SIMD is applied
- Compilers do not cut the cheese
- Method adaptable to other applications (e.g., other high-precision reductions, data corruption checks)



Example: Energy analysis of KPM

- Time to solution has lowest-order impact on energy
- Tailored kernels are key to performance (4.5x in runtime & energy)
- Energy-performance models yield correct qualitative insight
- Future: Large-scale energy analysis & modeling



$$E(n) = F \cdot \frac{W_{00} + n(W_{01} + W_1 f + W_2 f^2)}{\min(nP_0(f), P_{\max})}$$

Energy-performance model

Download our building block library and applications:

`http://tiny.cc/ghost`

GHOST *General, Hybrid, and Optimized Sparse Toolkit*

Thank you.

SPPEXA