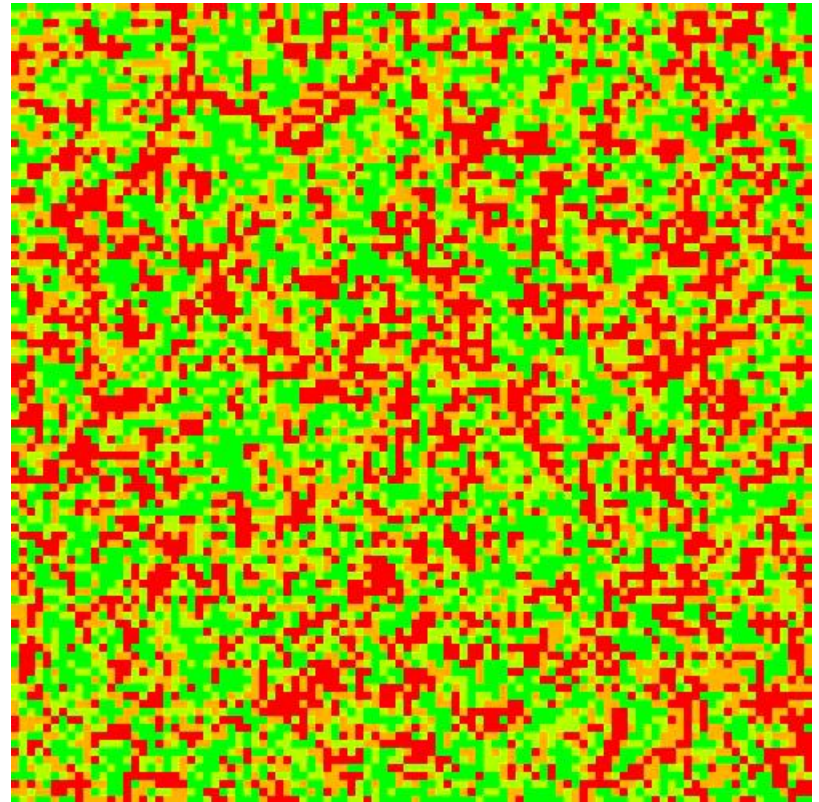
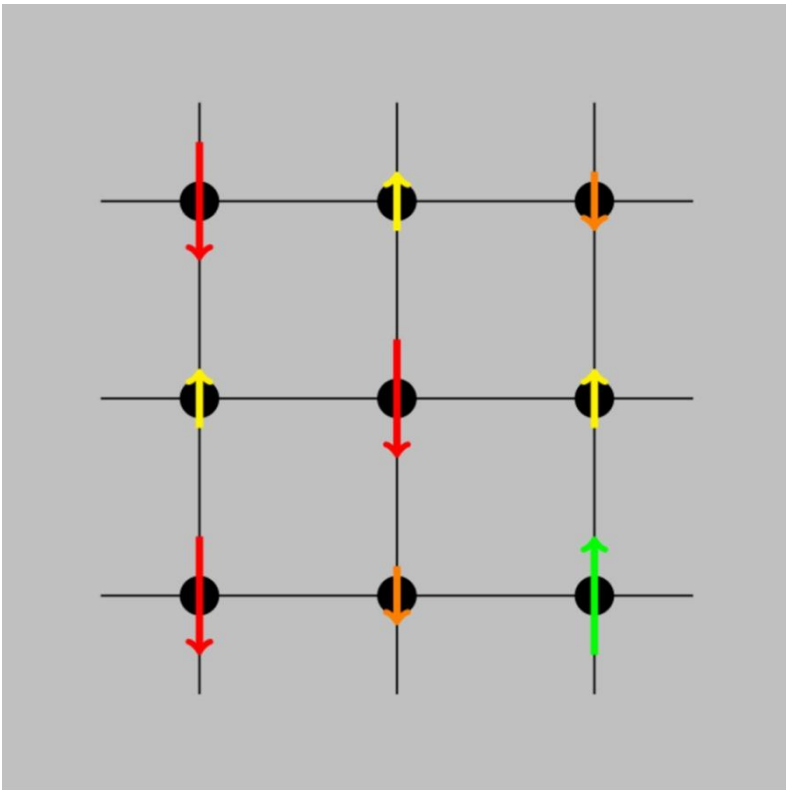


# Monte Carlo / Metropolis for the Potts model

Mario Könz / Dominik Gresch

# Physical Problem

## 3D, 4-states Potts Model



# Metropolis algorithm

## Steps

- select random spin
- select random direction of change
- calculate energy difference

$$\Delta E_i = J \cdot \sum_{j \in \text{neighbours}} \sigma_i \cdot \sigma_j$$

- accept change with probability

$$p_i = \min \left[ 1, \exp \left( -\frac{\Delta E_i}{k_B T} \right) \right]$$

## Computation

- RNG
- RNG
- memory access,  
periodic boundary
- RNG, exponential

# Modules

## SIM

- metropolis algorithm
- measurement
- contains GRID & RNG

## GRID

- boundary condition
- contains MATRIX

## MATRIX

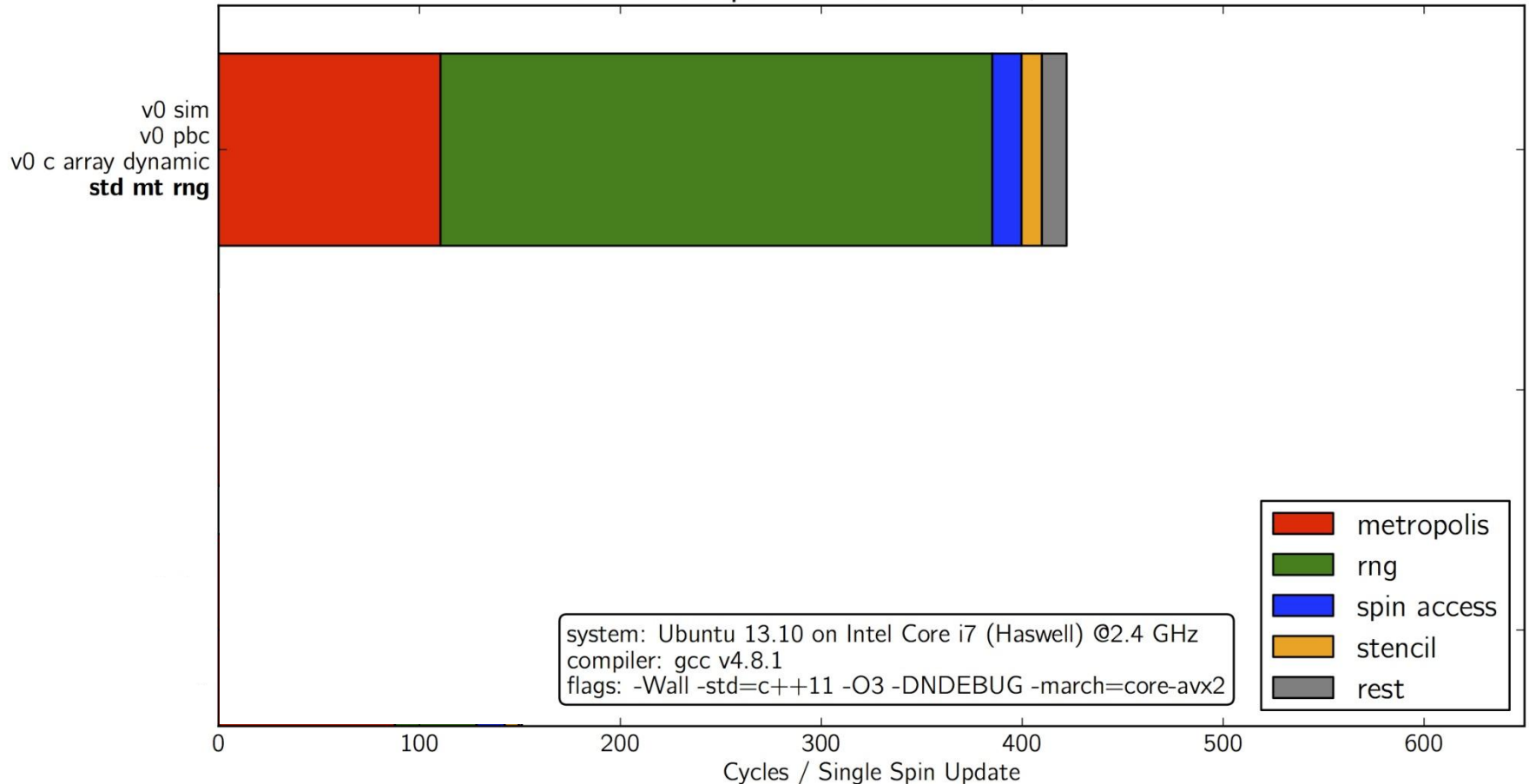
- storage format of spins
- handles data type and ordering

## RNG

- MT19937

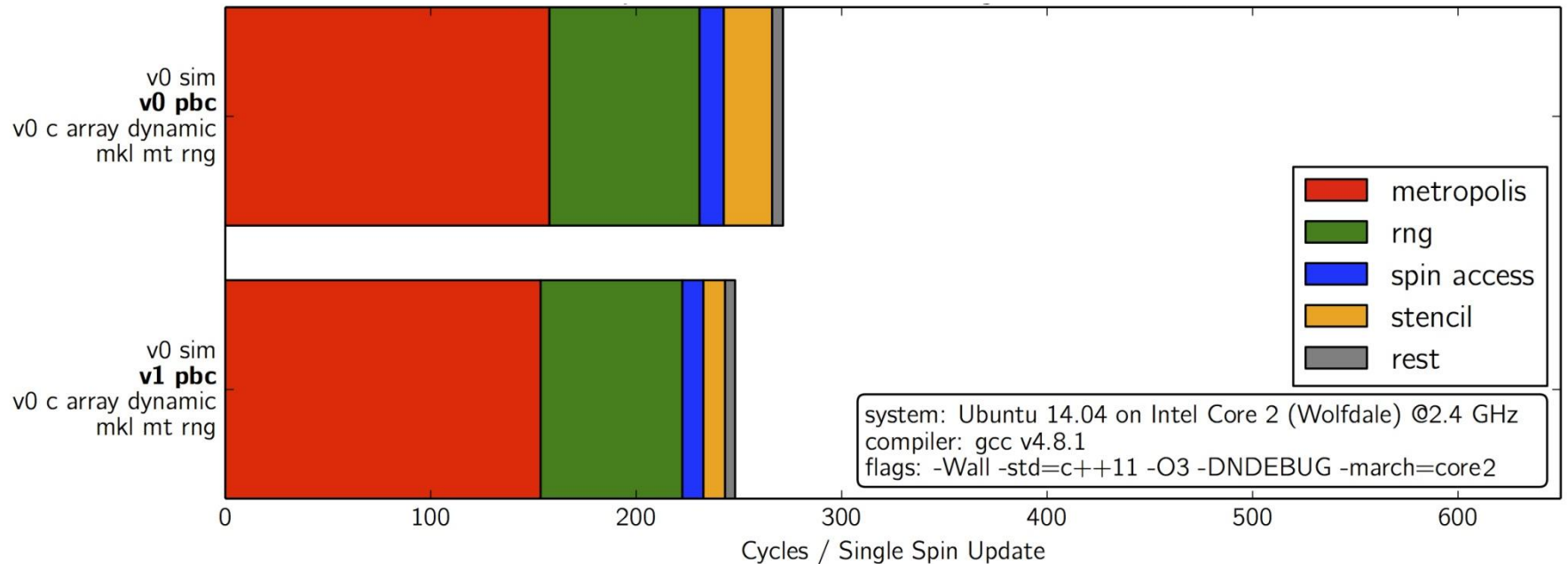
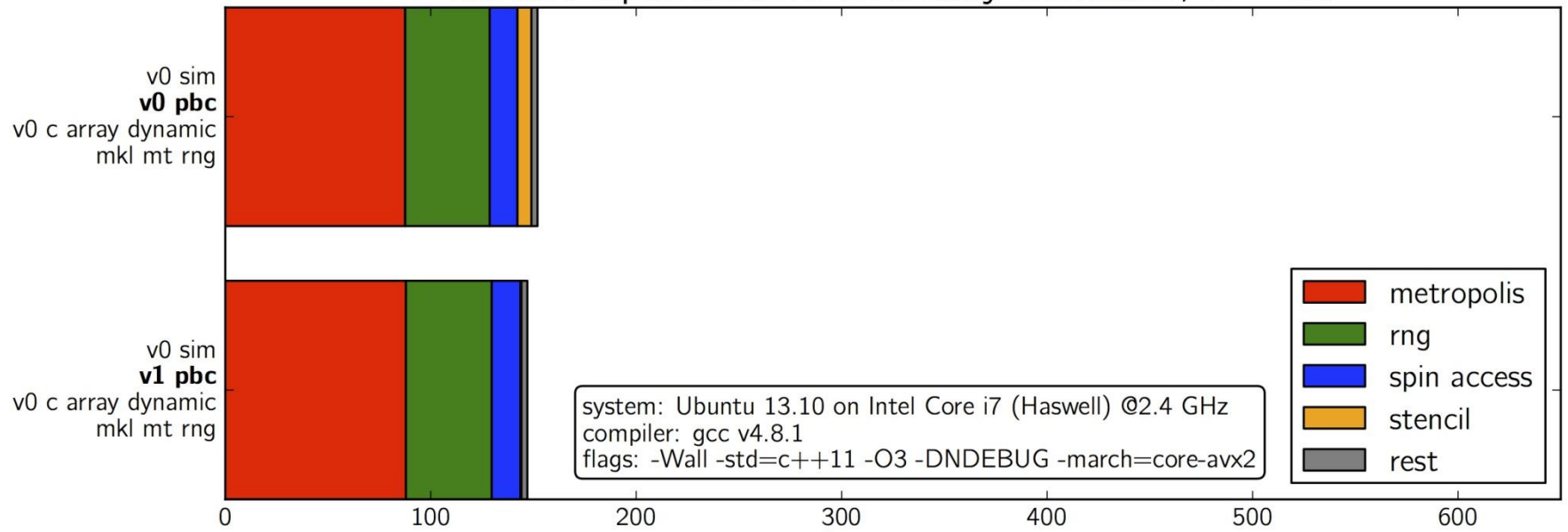
# economic RNG usage / MKL

Module Optimization: RNG, N = 20



**boundary condition lookup table**

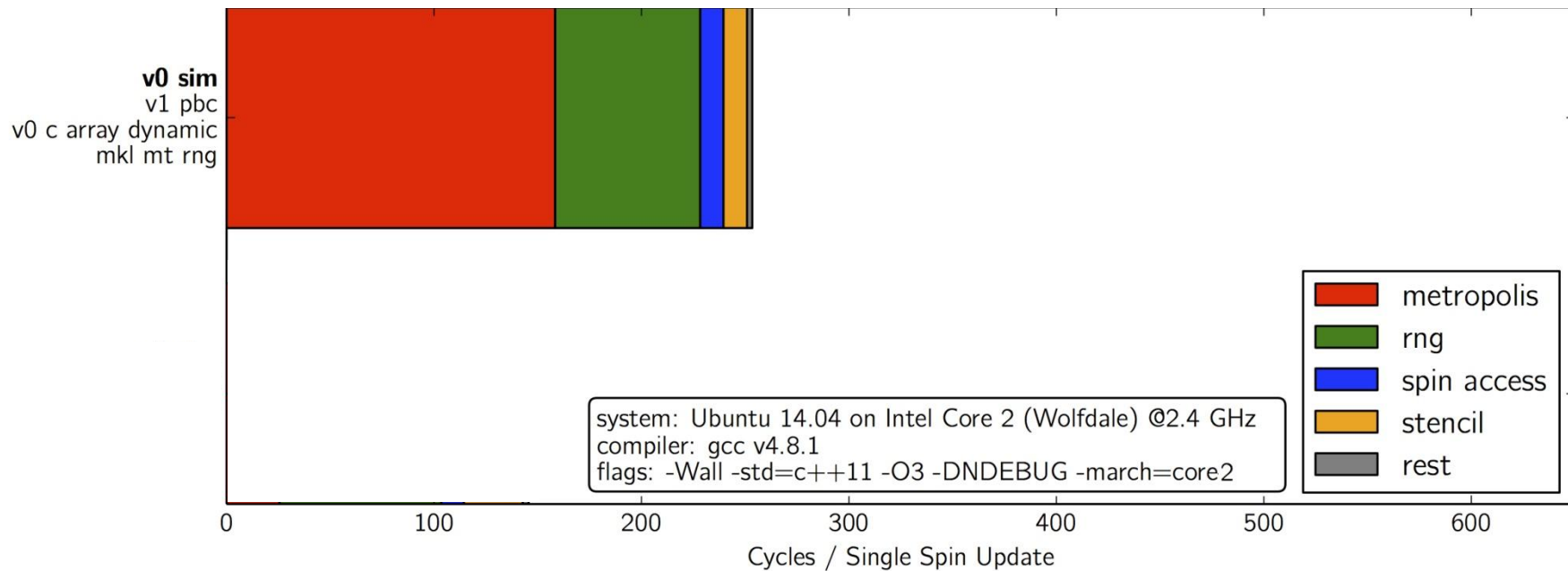
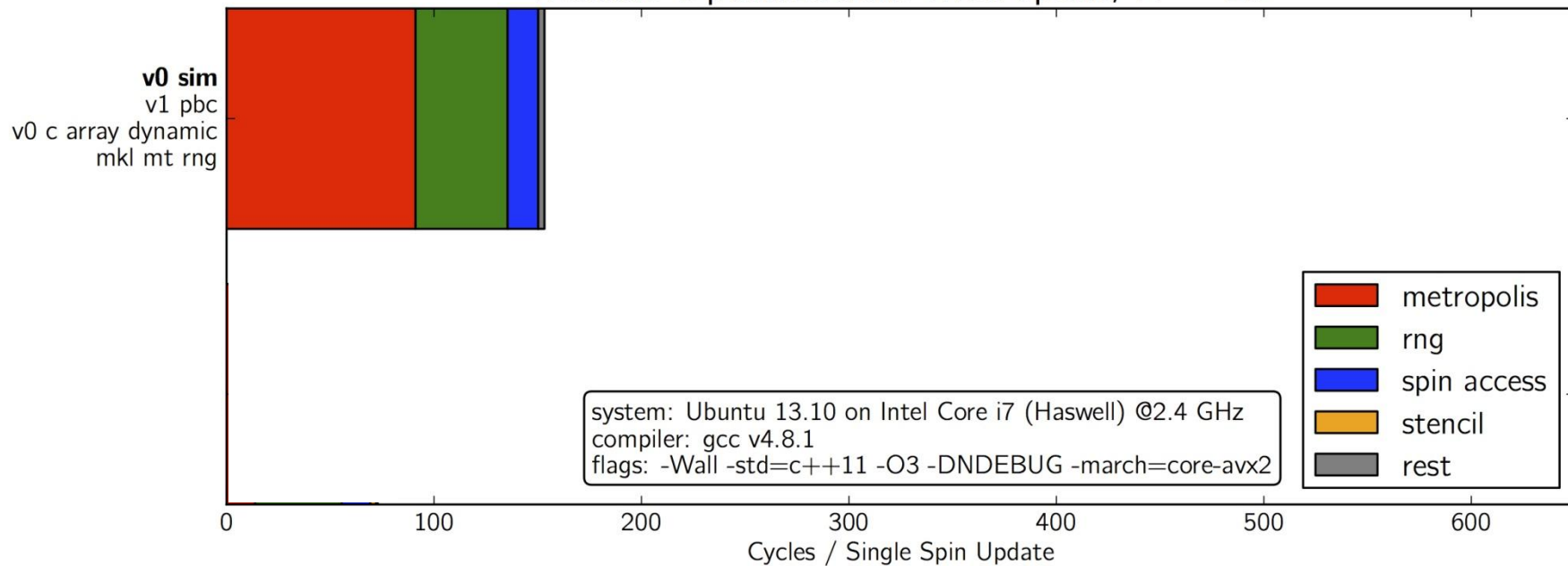
# Module Optimization: Boundary Condition, $N = 20$



**precompute exponentials**

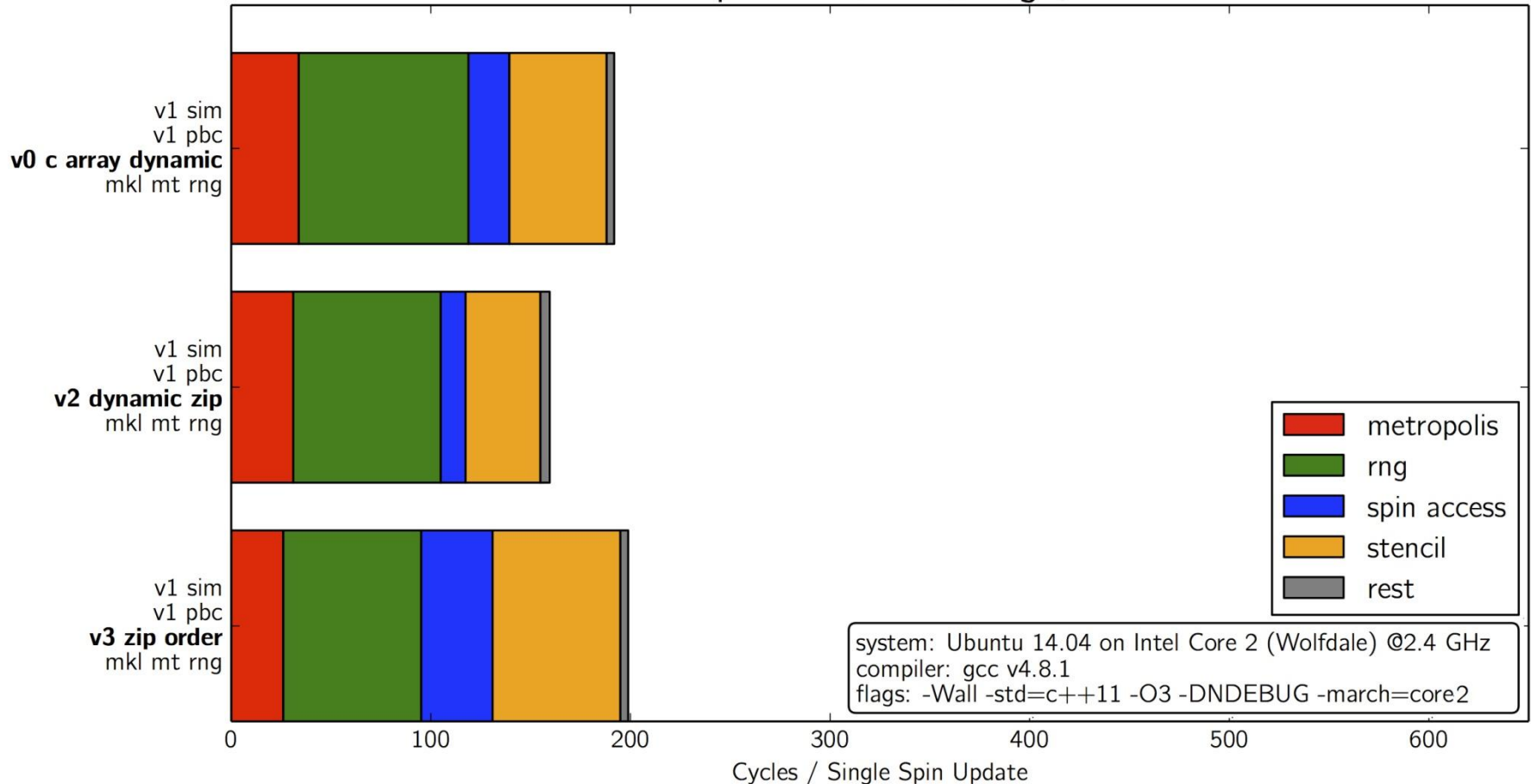


## Module Optimization: Metropolis, N = 20



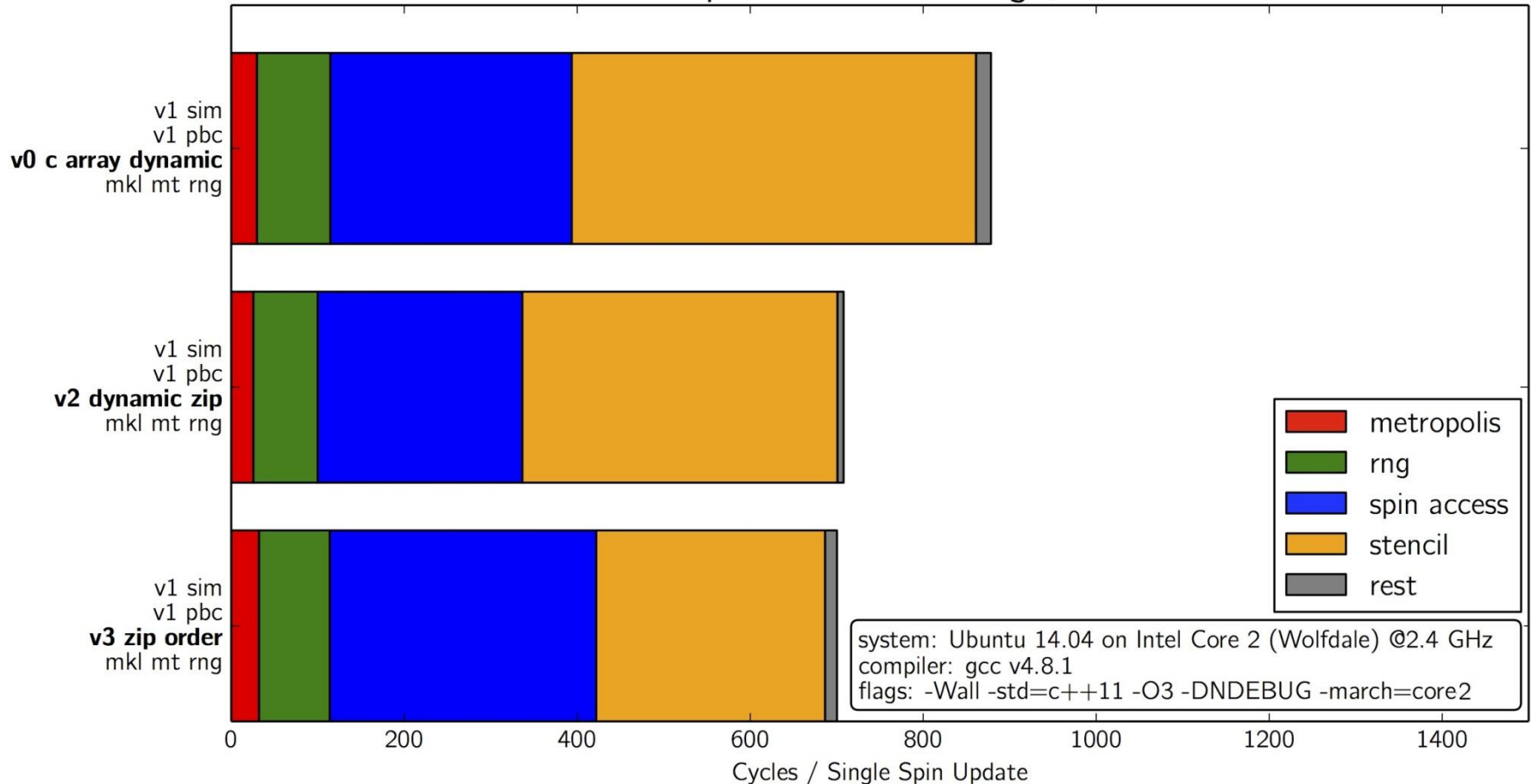
# compression / Z-order

Module Optimization: Storage, N = 20



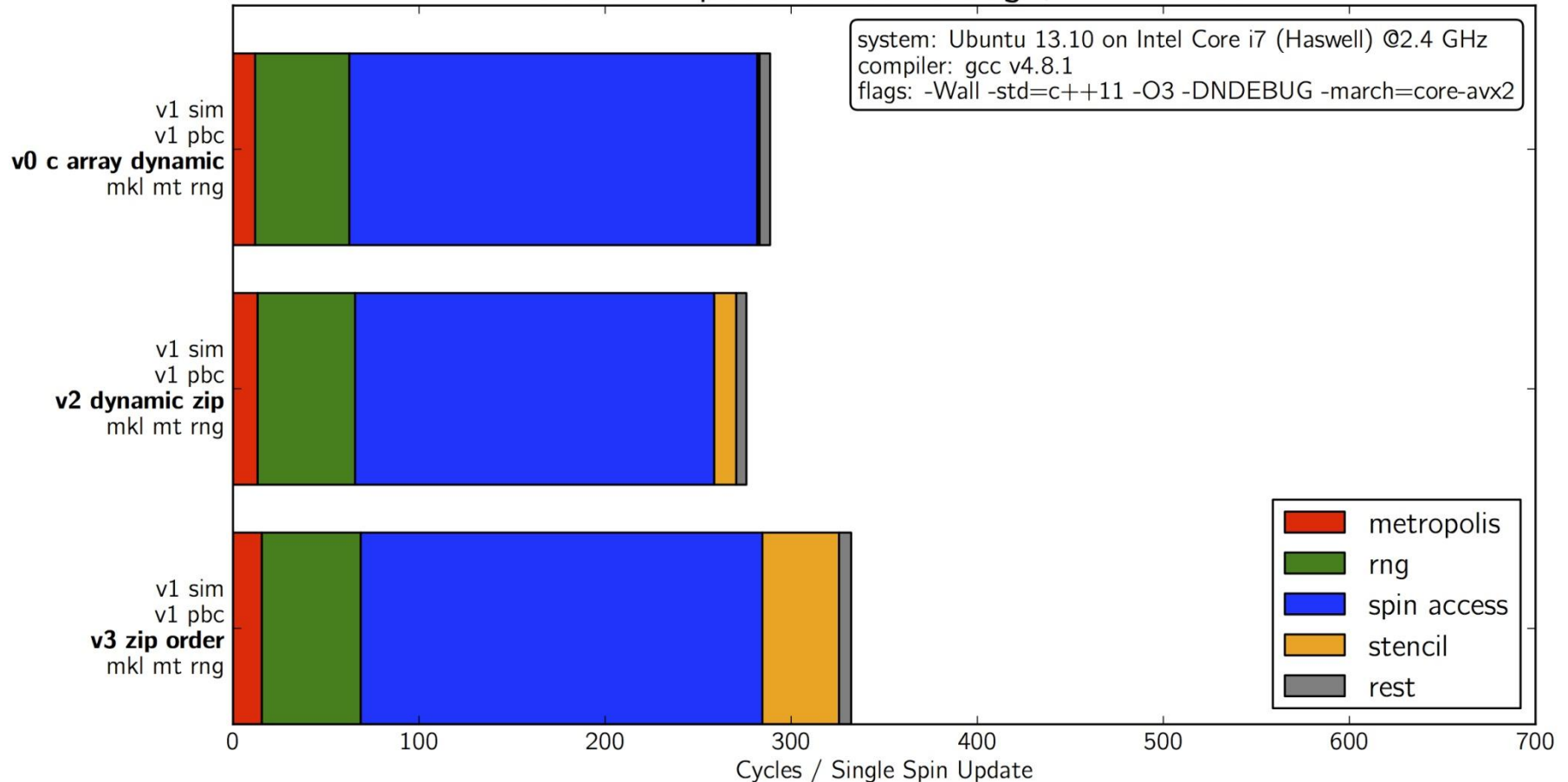
# compression / Z-order

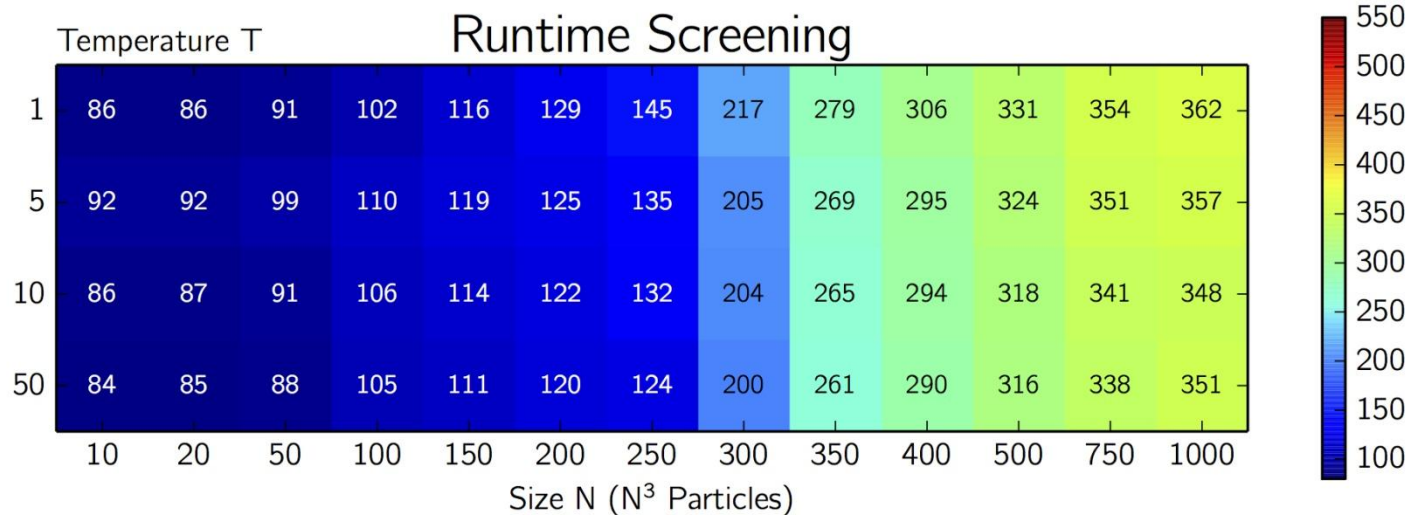
Module Optimization: Storage, N = 300



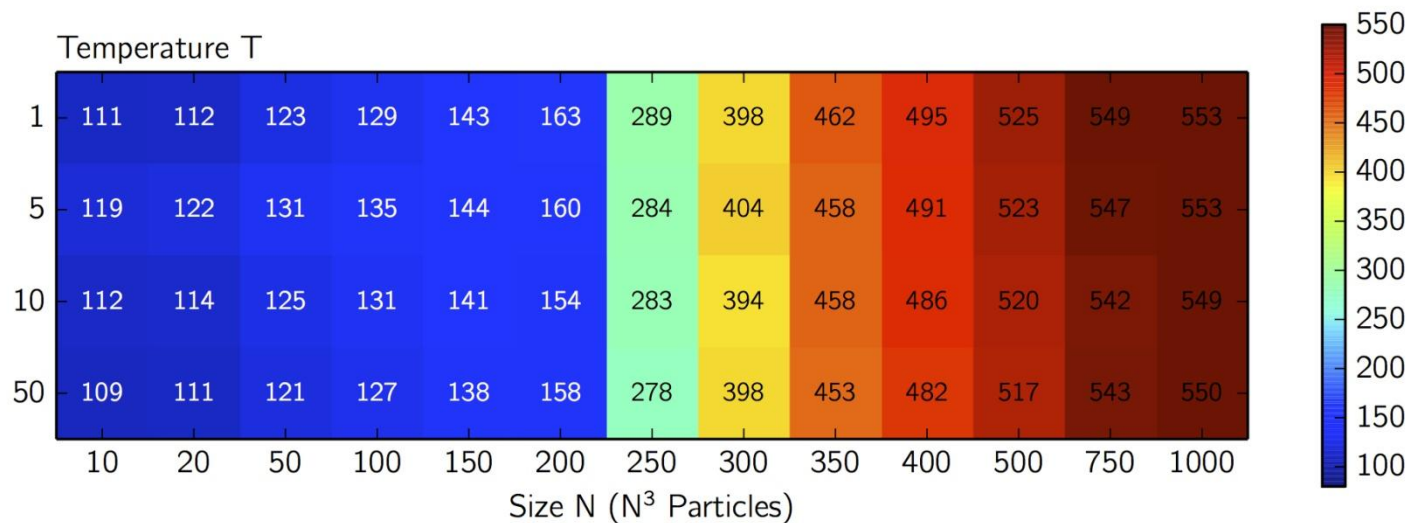
# Haswell prefetching?

## Module Optimization: Storage, $N = 1000$

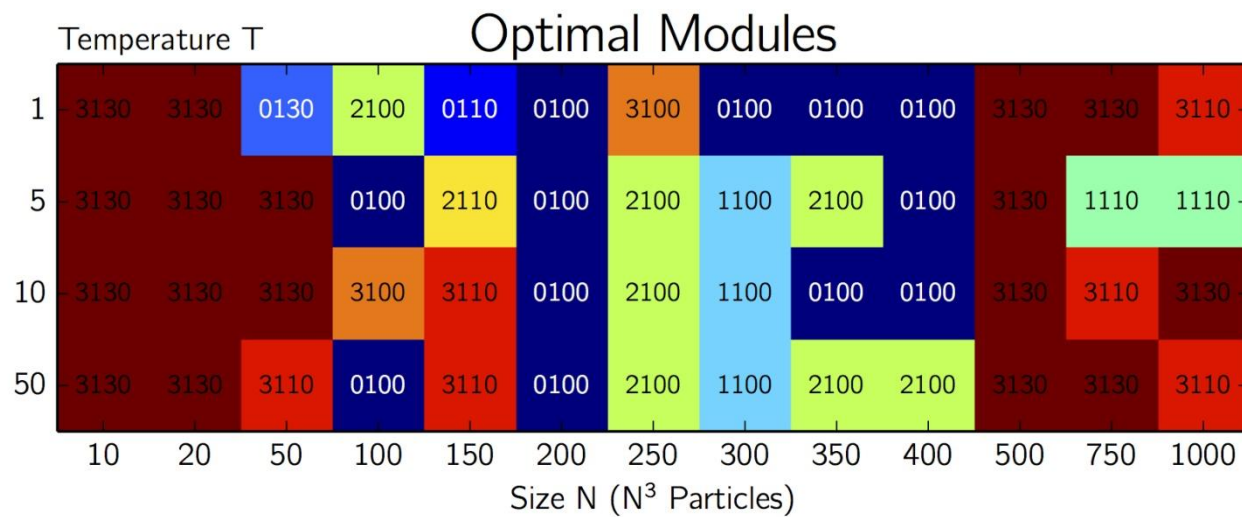




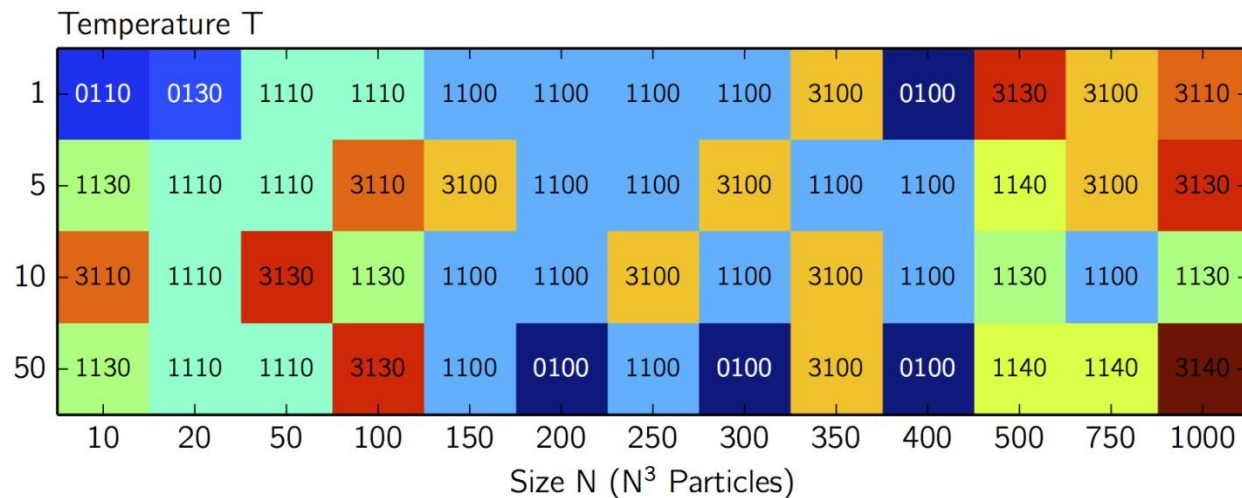
system: Ubuntu 13.10 on Intel Core i7 (Haswell) @2.4 GHz  
compiler: gcc v4.8.1  
flags: -Wall -std=c++11 -O3 -DNDEBUG -march=core-avx2



system: Ubuntu 14.04 on Intel Core 2 (Wolfdale) @2.4 GHz  
compiler: gcc v4.8.1  
flags: -Wall -std=c++11 -O3 -DNDEBUG -march=core2



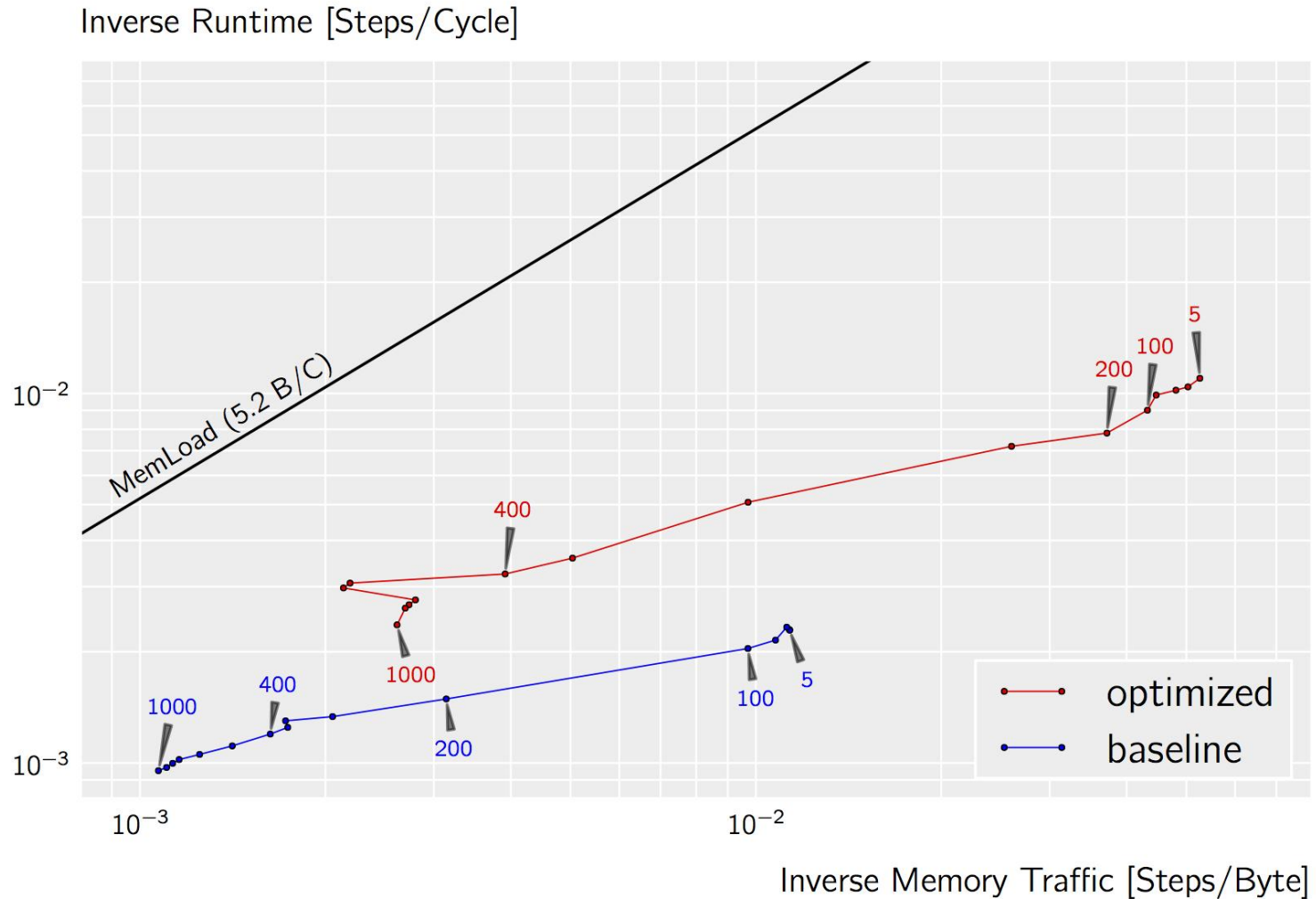
Haswell



Wolfdale

0: greschd v6 sim / 1: greschd v2 sim / 2: greschd v4 sim / 3: greschd v3 sim  
 1: msk v1 pbc  
 0: msk v2 dynamic zip / 1: msk v0 std vec / 3: msk v0 c array dynamic / 4: msk v3 zip order  
 0: mkl mt rng

# Roofline Plot



system: Ubuntu 13.10 on Intel Core i7 (Haswell) @2.4 GHz  
compiler: gcc v4.8.1  
flags: -Wall -std=c++11 -O3 -DNDEBUG -march=core-avx2

**Thank you for your Attention**

**Questions?**