Rethinking the Parallelization of Random-Restart Hill Climbing

A Case Study in Optimizing a 2-Opt TSP Solver for GPU Execution

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Overview

- TSP and 2-opt heuristic
- Previous GPU approaches
  - Assign a climber per thread
- Our new approach
  - Assigns a climber per thread block, parallelizes the 2-opt evaluations between threads in a block
  - Several other optimizations
  - Outperforms previous implementations
- Experimental comparison

Traveling Salesman Problem (TSP)

- Combinatorial optimization problem
  - Find minimum-distance Hamiltonian tour in complete, undirected, weighted graph
  - Finding optimal solution is NP-hard
  - Test bed for heuristic approximation approaches
- Application areas
  - Logistics
  - Wire routing
  - Genome analysis

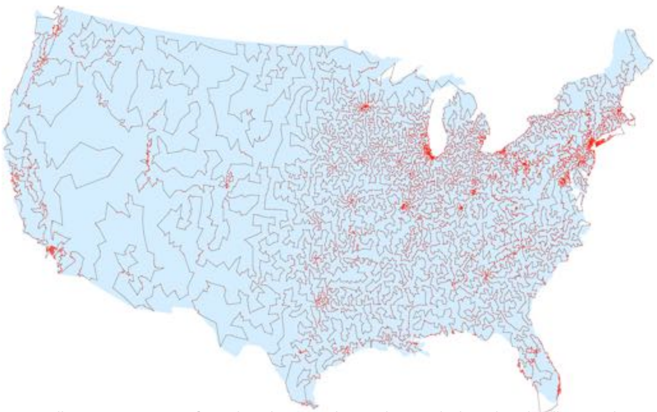


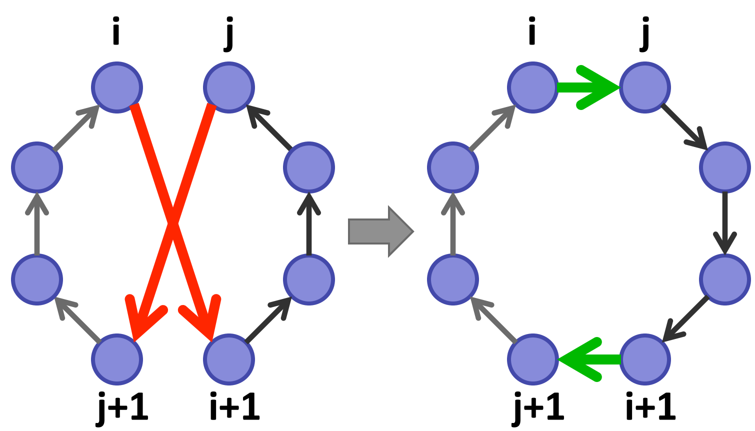
Illustration courtesy of David Applegate, Robert Bixby, Vasek Chvatal, and William Cook

Random-Restart Hill Climbing

- Iterative hill climbing (IHC) local search
  - Generate initial candidate solution
  - Iteratively improve solution via move to neighbor
  - Unlikely to reach global optimum
- Random restart
  - Repeatedly perform IHC from random initial solutions
  - Can require 1,000s to 1,000,000s+ of restarts
  - Each restart (*climber*) is independent; evaluation of possible moves within each climber also independent

2-Opt Move Evaluation

- Random-restart TSP
  - Generate *k* random initial tours (city orderings)
  - Iteratively improve tours until local minimum reached
- Tour improvement via application of *2-opt move*
  - Remove edges (**i**,**i+1**) and (**j**,**j+1**) of the tour, reconnect the resulting subtours in the other order by adding edges (**i**,**j**) and (**i+1**,**j+1**)



  - In each IHC step, evaluate all moves and apply best

2-opt Pseudo Code

```
// city[i] is ith city in tour order
#define dist(a,b) dmat[city[a]][city[b]]
do {
  minchange = 0
  for (i = 0; i < cities-2; i++) {
    for (j = i+2; j < cities; j++) {
      change = dist(i,j) + dist(i+1,j+1)
               - dist(i,i+1) - dist(j,j+1)
      if (minchange > change) {
        minchange = change
        mini = i, minj = j
      } } }
  // apply best 2-opt move (mini/minj)
} while (minchange < 0)
```

Distance matrix: O(n^2) time/space

Don't evaluate symmetric or adjacent edges

No need to compute actual tour length

2-opt Pseudo Code

```
// city[i] is ith city in tour order
#define dist(a,b) dmat[city[a]][city[b]]
do {
  minchange = 0
  for (i = 0; i < cities-2; i++) {
    minchange += dist(i,i+1)
    for (j = i+2; j < cities; j++) {
      change = dist(i,j) + dist(i+1,j+1) - dist(j,j+1)
      if (minchange > change) {
        minchange = change
        mini = i, minj = j
      } }
    minchange -= dist(i,i+1)
  }
  // apply best 2-opt move (mini/minj)
} while (minchange < 0)
```

Pull loop-invariant edge out of inner j-loop

Experimental Methodology

- Metric
  - Throughput in billions of 2-opt moves evaluated per second (*Gigamoves*/second)
- System
  - K40 (Kepler) GPU with 15 SMs and 2880 PEs
  - TACC Maverick node (2x Xeons with 10 cores each)
- Inputs
  - First *n* points of 'd18512.tsp' from TSPLIB
  - Select climber count *k* to fully load SMs

1. Distance Matrix (*matr_s*)

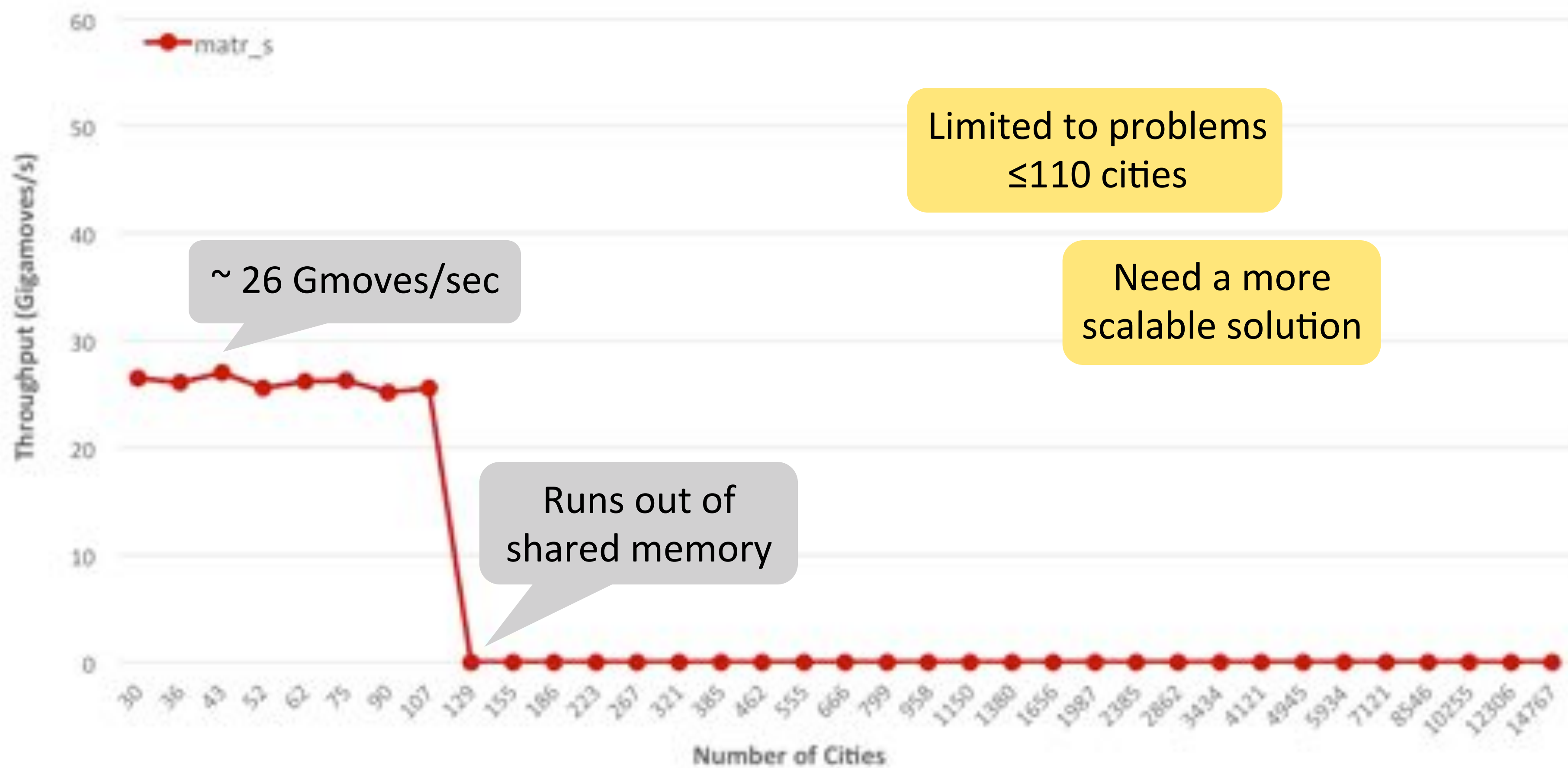
- Our original implementation (2011)
  - Assign a climber (initial random tour) per thread
  - Pre-compute distance matrix in shared memory
  - Each climber needs a tour order array (local memory)

✔ Distance lookups all to shared memory

✖ O(n^2) shared memory requirement (48kB max) limits problem size to 110 cities

✖ Lots of bank conflicts from random matrix accesses

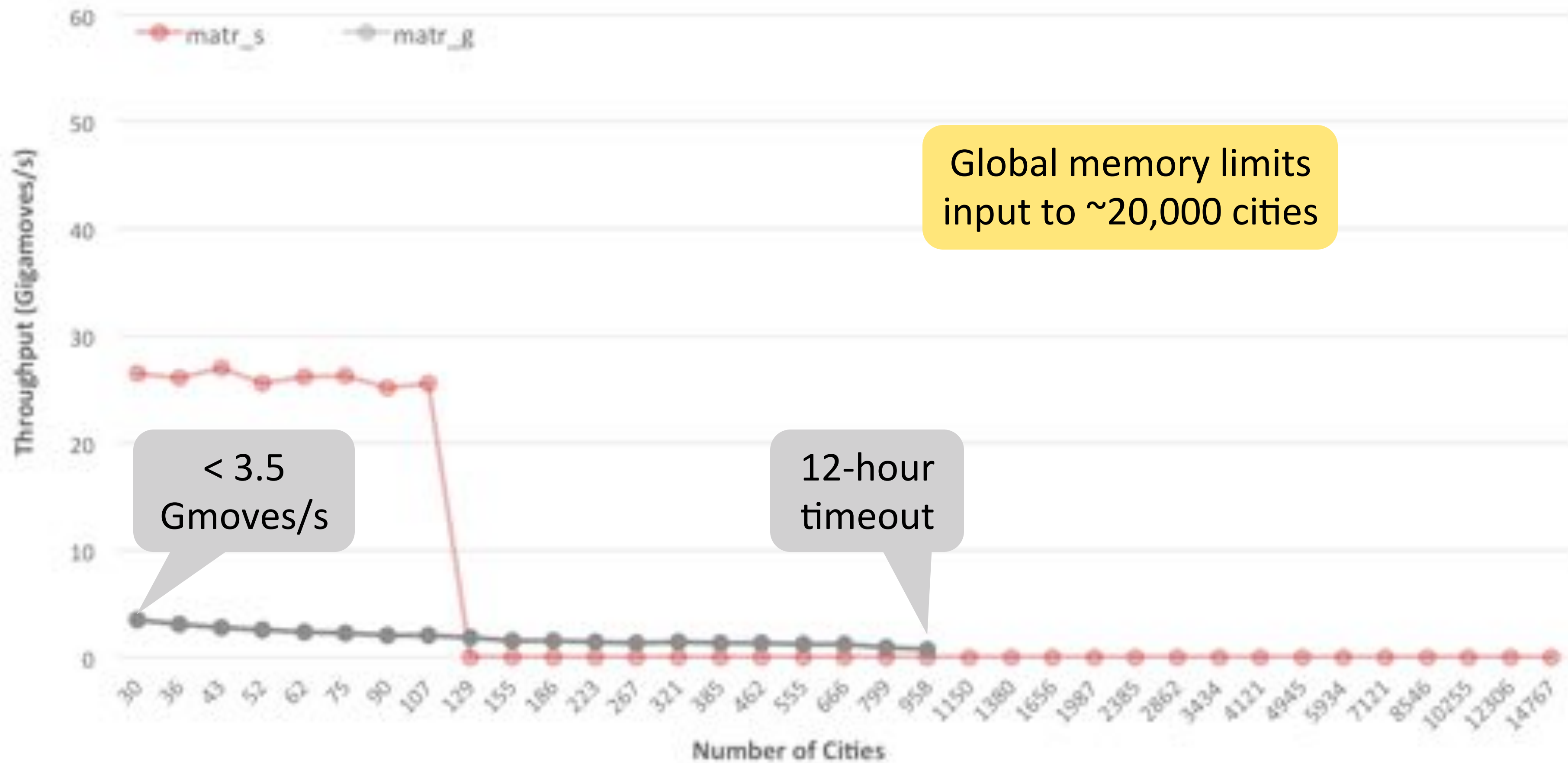
Throughput: *matr_s*



2. Distance Matrix—Global (*matr_g*)

- Naïve way to remove the shared mem limit…
  - Pre-compute distance matrix in global memory
  - ✔ No more shared memory limit on problem size
  - ✖ Random accesses to large global memory matrix are uncoalesced and uncached in the L1

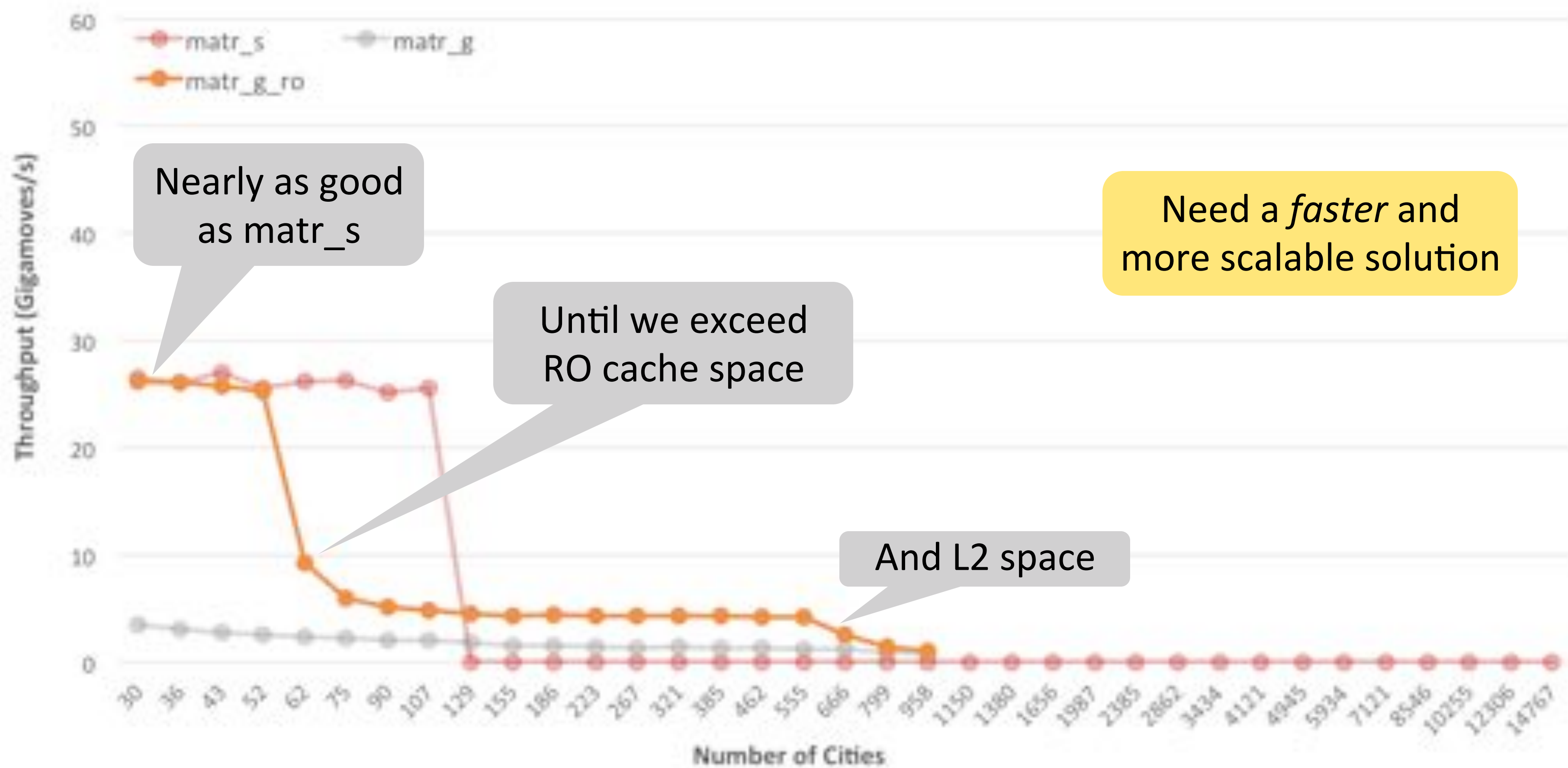
Throughput: *matr_g*



2. Distance Matrix—Global (*matr_g_ro*)

- ~~Naïve way to remove the shared mem limit…~~
  - ~~Pre-compute distance matrix in global memory~~
  - ~~✔ No more shared memory limit on problem size~~
  - ~~✖ Random accesses to large global memory matrix are uncoalesced and uncached in the L1~~
- OK, but distance matrix is read-only…
  - Use __*ldg()* to force read onto read-only data cache path
  - ✔ High hit rate in the cache at smaller problem sizes
  - ✖ Still random access pattern to O(n^2) storage

Throughput: *matr_g_ro*



3. Distance Re-Calculation (*calc*)

- Published by K. Rocki and R. Suda (2012, 2013)
  - Re-compute distances as needed rather than look up
  - Allows direct permutation of coordinates in tour order (no need for separate array)

✔ O(*n*) storage allows larger problem sizes (~4000)

✔ Coalesced memory accesses

✖ Limited by local memory size

✖ Large *k* (≥30720) needed to fully utilize K40 GPU

Pseudo Code Update

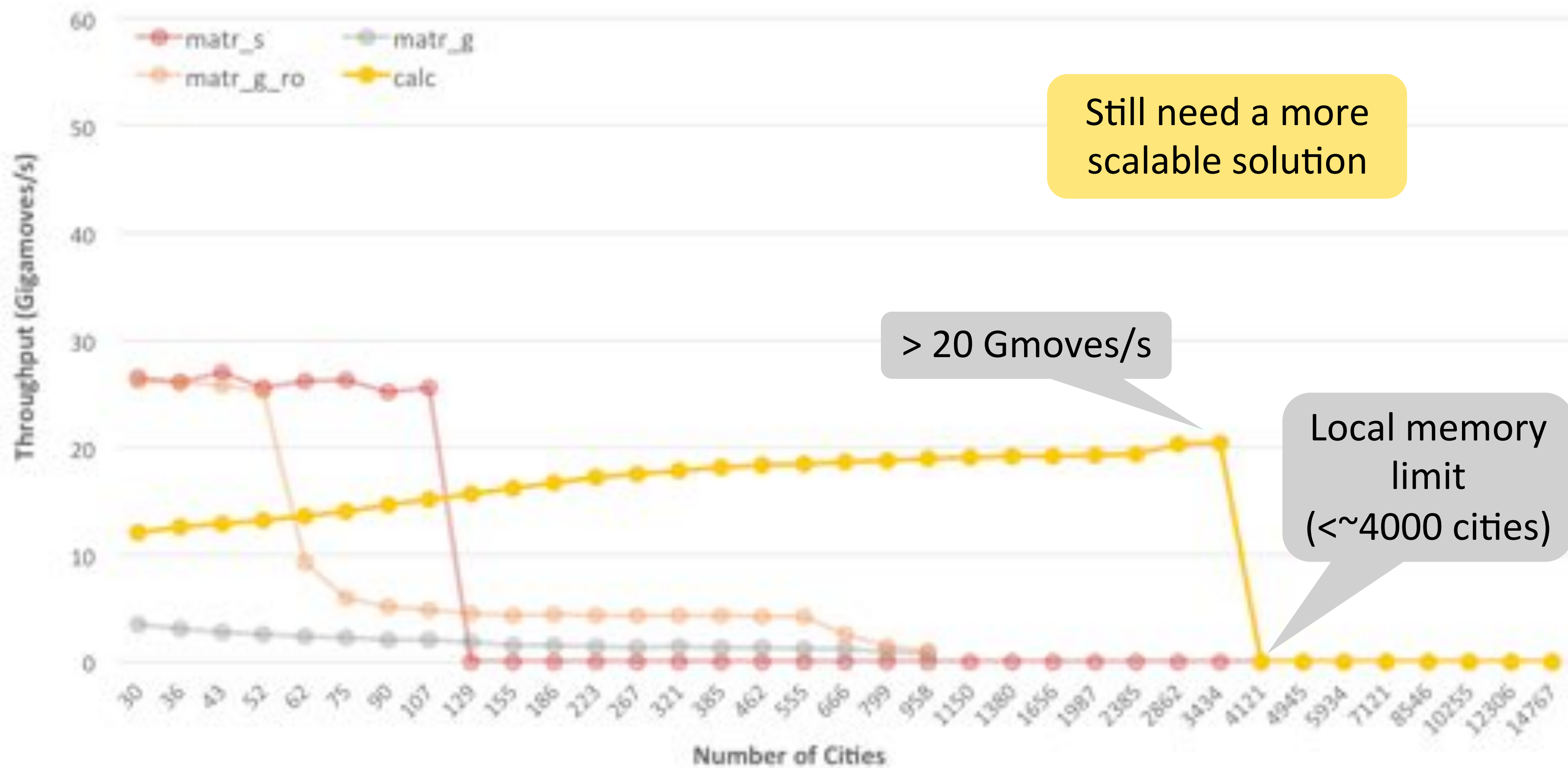
```
// city[i] is ith city in tour order
#define dist(a,b) dmat[city[a]][city[b]]
do {
  minchange = 0
  for (i = 0; i < cities-2; i++) {
    minchange += dist(i,i+1)
    for (j = i+2; j < cities; j++) {
      change = dist(i,j) + dist(i+1,j+1) - dist(j,j+1)
      if (minchange > change) {
        minchange = change
        mini = i, minj = j
      } }
    minchange -= dist(i,i+1)
  }
  // apply best 2-opt move (mini/minj)
} while (minchange < 0)
```

Pseudo Code Update

```
// x[i],y[i] are coordinates of ith city in tour order
#define dist(a,b) sqrtf( (x[a]-x[b])2 + (y[a]-y[b])2 )
do {
  minchange = 0
  for (i = 0; i < cities-2; i++) {
    minchange += dist(i,i+1)
    for (j = i+2; j < cities; j++) {
      change = dist(i,j) + dist(i+1,j+1) - dist(j,j+1)
      if (minchange > change) {
        minchange = change
        mini = i, minj = j
      } }
    minchange -= dist(i,i+1)
  }
  // apply best 2-opt move (mini/minj)
} while (minchange < 0)
```

Re-calculate distance rather than index into matrix

Throughput: *calc*



4. Intra-Parallelization (*intra*)

- Hierarchical parallelization of the 2-opt evals
  - Assign a tour per thread block instead of per thread
  - Parallelize 2-opt computation across threads in block
    - Distribute outer i-loop across threads in block (fully parallelized if cities < 1024); inner j-loop sequential
    - Requires reduction + sync to identify best 2-opt move

✔ Storage requirement per block reduced

- Single set of coordinates in tour order

✖ Complexity of implementation increases

Pseudo Code Update—Intra

```
#define dist(a,b) sqrtf( (x[a]-x[b])^2 + (y[a]-y[b])^2 )
do {
  minchange = 0
  for (i = 0; i < cities-2; i++) {
    minchange += dist(i,i+1)
    for (j = i+2; j < cities; j++) {
      change = dist(i,j) + dist(i+1,j+1) - dist(j,j+1)
      if (minchange > change) {
        minchange = change
        mini = i, minj = j
      } }
    minchange -= dist(i,i+1)
  }
  // apply best 2-opt move (mini/minj)
} while (minchange < 0)
```

Pseudo Code Update—Intra

```
#define dist(a,b) sqrtf( (x[a]-x[b])^2 + (y[a]-y[b])^2 )
do {
  minchange = 0
  for (i = threadID; i < cities-2; i += blockDim) {
    minchange += dist(i,i+1)
    for (j = i+2; j < cities; j++) {
      change = dist(i,j) + dist(i+1,j+1) - dist(j,j+1)
      if (minchange > change) {
        minchange = change
        mini = i, minj = j
      } }
    minchange -= dist(i,i+1)
  }
  __syncthreads()
  // reduction to identify + apply best 2-opt move
} while (minchange < 0)
```

Distribute outer loop to threads in block

Each thread tracks its best move; reduction required to find overall best

Pseudo Code Update—Intra

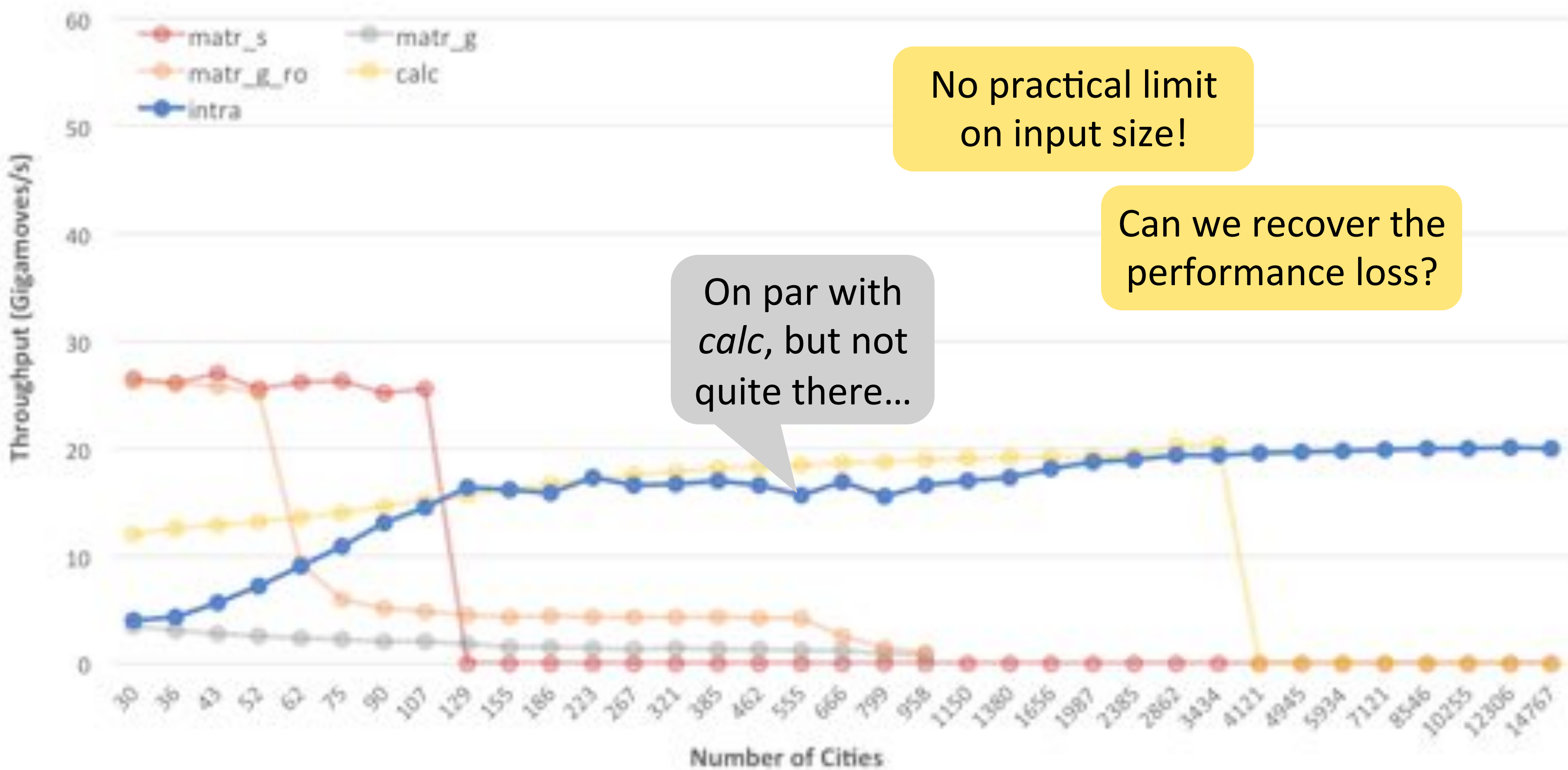
```
#define dist(a,b) sqrtf( (x[a]-x[b])² + (y[a]-y[b])² )
do {
  for (i = threadID; i < cities; i += blockDim)
    buf[i] = -dist(i,i+1)
  __synchthreads()

  minchange = 0
  for (i = threadID; i < cities-2; i += blockDim) {
    minchange -= buf[i]
    for (j = i+2; j < cities; j++) {
      change = dist(i,j) + dist(i+1,j+1) + buf[j]
      if (minchange > change) {
        minchange = change
        mini = i, minj = j
      } }
    minchange += buf[i]
  }
  __synchthreads()
  // reduction to identify + apply best 2-opt move
} while (minchange < 0)
```

Pre-compute tour segment lengths

Segment distances read from global memory buffer

Throughput: *intra*



No practical limit on input size!

Can we recover the performance loss?

On par with *calc*, but not quite there…

5. Intra-Parallelization + ShMem Tiling (*tile*)

- Blocks share ordered tour and buffer space
  - Shared mem is small, don't want to limit problem size
- Strip mine the inner j-loop
  - Break iterations into chunks s.t. each chunk's working set fits in shared memory and preload each tile
  - But… each thread's j-loop begins at a different index!
    - Solution: run inner j-loop backwards

✔ Most accesses go to shared memory

✔ No bank conflicts, full coalescing

✖ Implementation complexity increases further

Pseudo Code Update—Tile

```
for (j = i+2; j < cities; j++) {
  change = dist(i,j) + dist(i+1,j+1)
           + buf[j]
  if (minchange > change) {
    minchange = change
    mini = i, minj = j
  }
}
```

Pseudo Code Update—Tile

Run inner loop in reverse to align initial *j* across threads

```
for (j = jj; j >= tileLowerBound; j--) {
  change = dist(i,j) + dist(i+1,j+1)
           + buf[j]
  if (minchange > change) {
    minchange = change
    mini = i, minj = j
  }
}
```

Pseudo Code Update—Tile

```
parallel_load_tile(x_shmem[], x[])
parallel_load_tile(y_shmem[], y[])
parallel_load_tile(buf_shmem[], buf[])
__syncthreads()

for (j = jj; j >= tileLowerBound; j--) {
  change = shmem_dist(i,j) + shmem_dist(i+1,j+1)
           + shmem_buf[j]
  if (minchange > change) {
    minchange = change
    mini = i, minj = j
  }
}
```

Coordinates and buffer now in shared memory

Pseudo Code Update—Tile

```
for (jj = cities-1; jj >= i+2; jj -= tileSize) {
  parallel_load_tile(x_shmem[], x[])
  parallel_load_tile(y_shmem[], y[])
  parallel_load_tile(buf_shmem[], buf[])
  __syncthreads()

  for (j = jj; j >= tileLowerBound; j--) {
    change = shmem_dist(i,j) + shmem_dist(i+1,j+1)
             + shmem_buf[j]
    if (minchange > change) {
      minchange = change
      mini = i, minj = j
    }
  }

}
```

J-loop broken into chunks, each pre-loads tile into shared memory

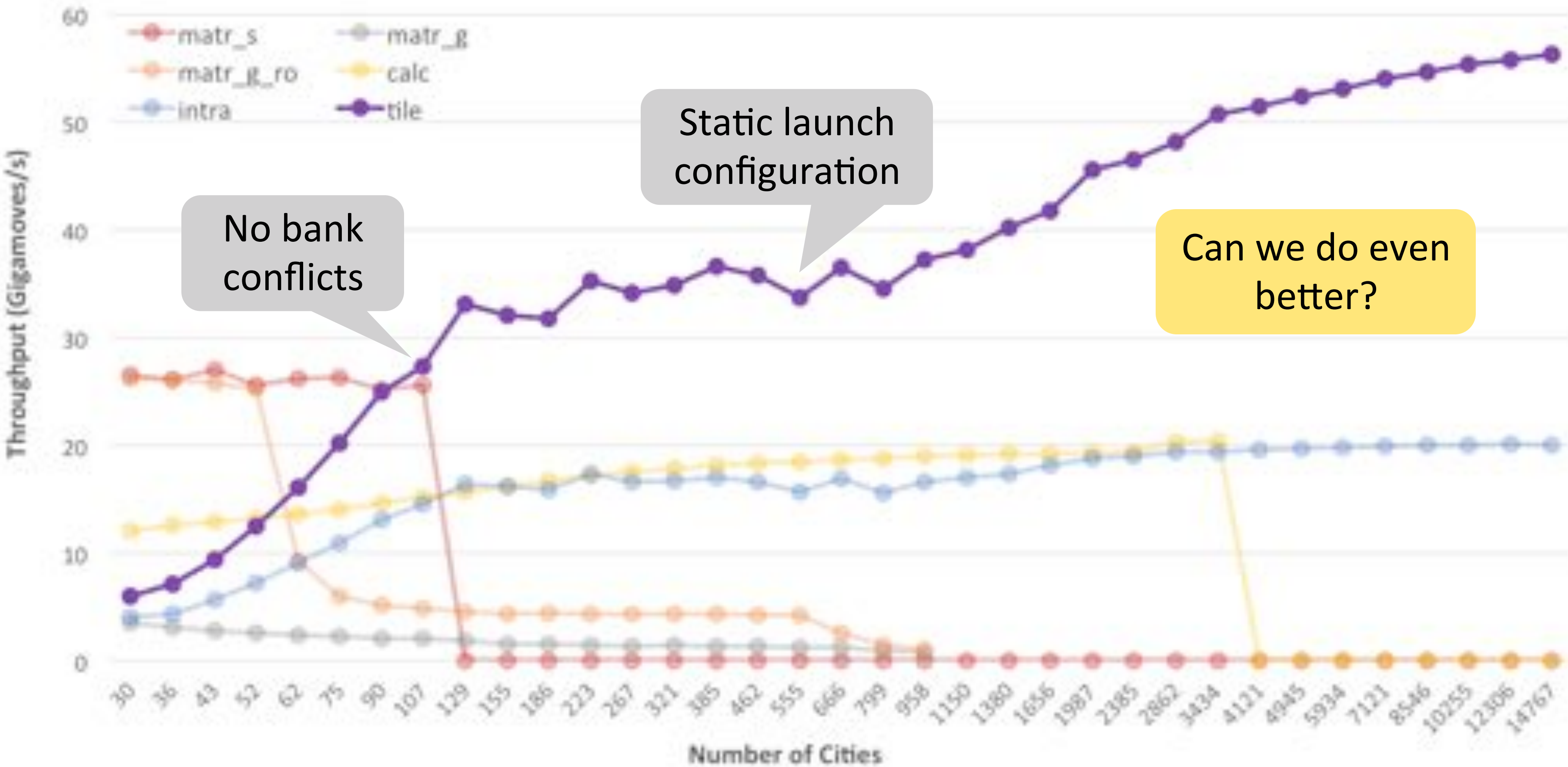
Pseudo Code Update—Tile

```
for (jj = cities-1; jj >= i+2; jj -= tileSize) {
  parallel_load_tile(x_shmem[], x[])
  parallel_load_tile(y_shmem[], y[])
  parallel_load_tile(buf_shmem[], buf[])
  __syncthreads()

  for (j = jj; j >= tileLowerBound; j--) {
    change = shmem_dist(i,j) + shmem_dist(i+1,j+1)
             + shmem_buf[j]
    if (minchange > change) {
      minchange = change
      mini = i, minj = j
    }
  }
  __syncthreads()
}
```

Additional synchronization

Throughput: *tile*



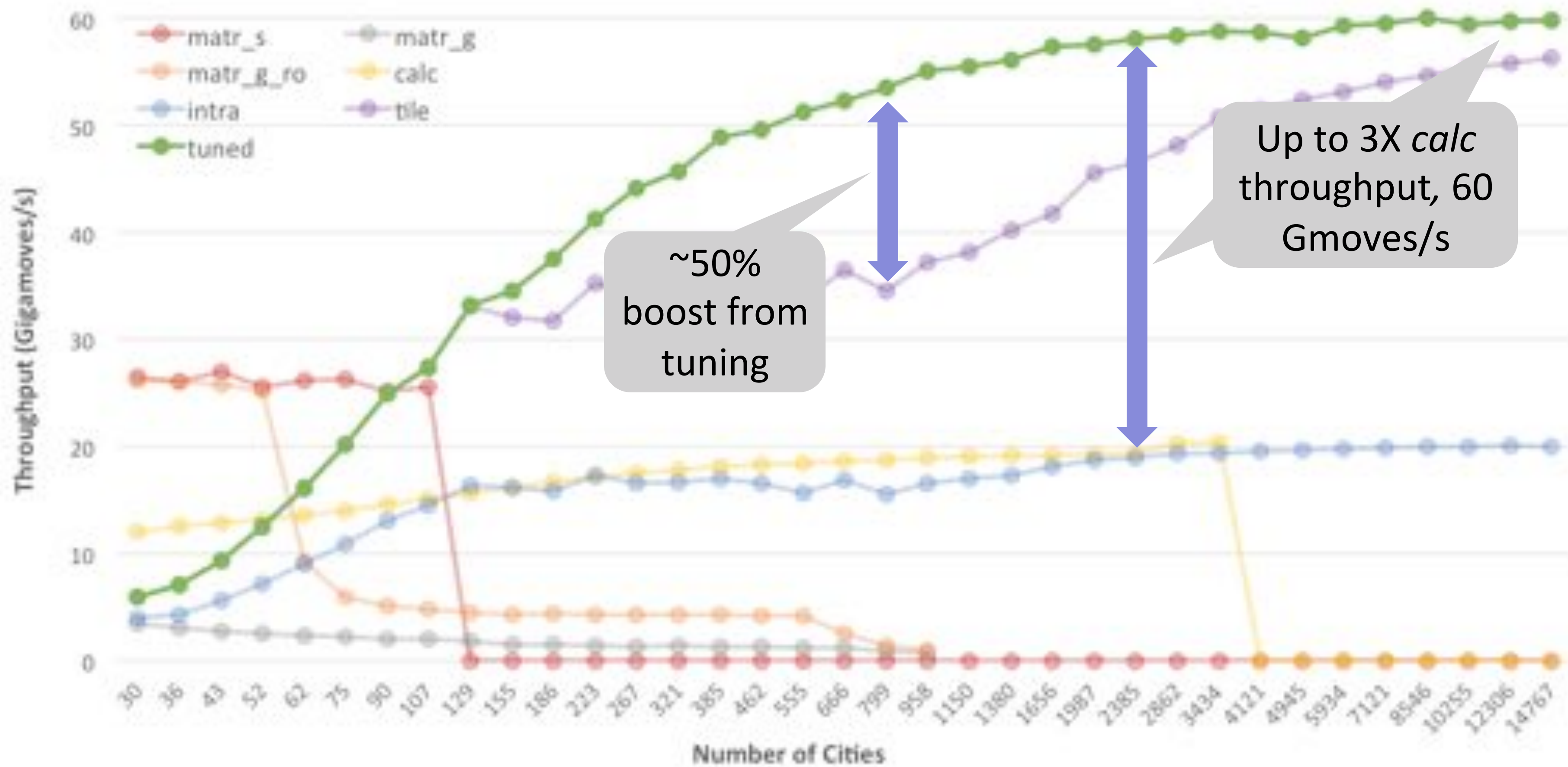
6. Intra + Tiling + Tuned Launch (*tuned*)

- Tune thread count per block
  - Based on # of cities, shared memory usage, max threads per block and SM, max blocks for SM, and registers per SM
- Launch kernel with computed thread count

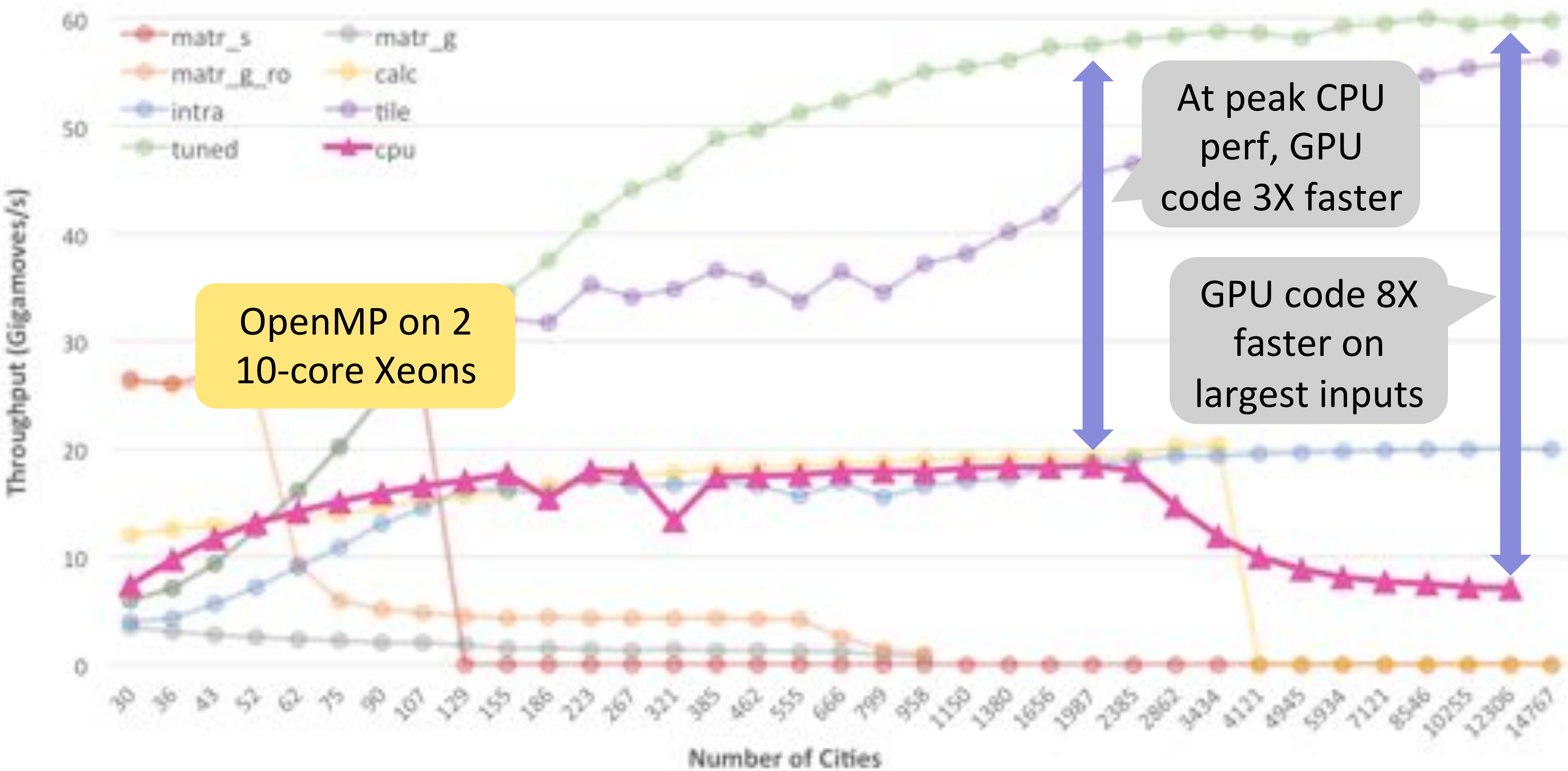
✔ Maximizes hardware usage

✖ None (except small CPU code block)

Throughput: *tuned*



Throughput: GPU vs. CPU



Conclusions

- CUDA 2-opt TSP solver based on hierarchical parallelization of climbers and move evaluation
  - Uses shared memory without limiting problem size
  - Faster time to first solution
  - Outperforms prior GPU implementations by up to 3X
  - Outperforms OpenMP version on 20 cores by up to 8X
- Another reminder to *rethink* parallelization strategy and optimize code for GPU hardware

Questions?

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