Blood Flow Simulation at Petascale and Beyond

Richard (Rich) Vuduc

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CS 267 Guest Lecture @ UC Berkeley

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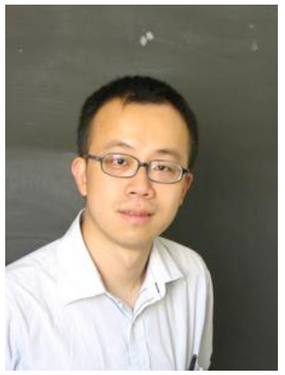

Lexing Ying

Aparna Chandramowlishwaran

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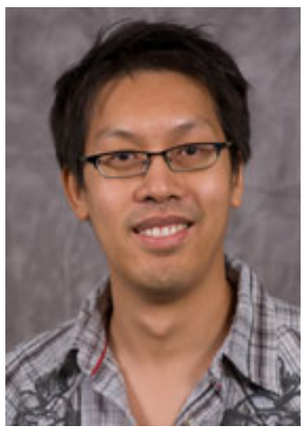

Rich Vuduc

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DARPA

DEPARTMENT OF ENERGY · UNITED STATES OF AMERICA ·

NVIDIA

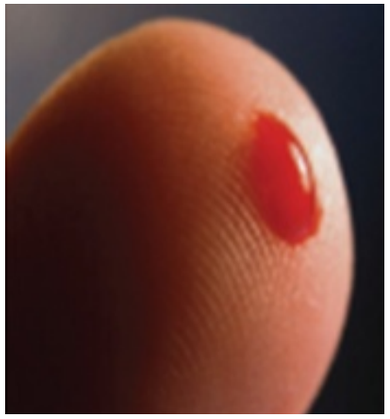
NATIONAL INSTITUTES OF HEALTH

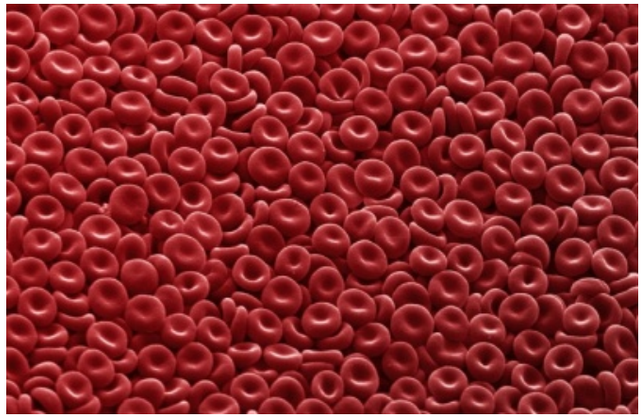
NSF

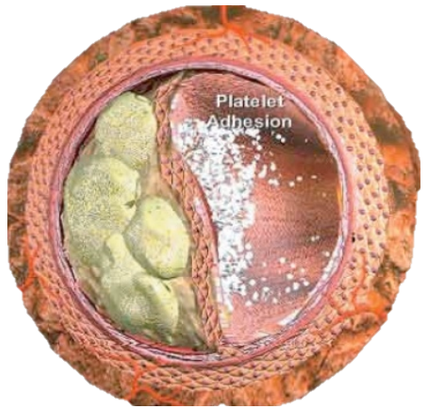
MARBLE OR GNOCCHI?

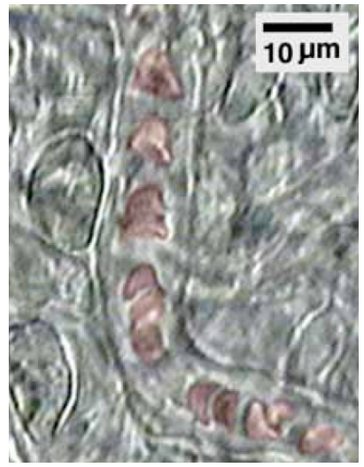
http://www.faqs.org/photo-dict/photofiles/list/2862/3795glass_marbles.jpg

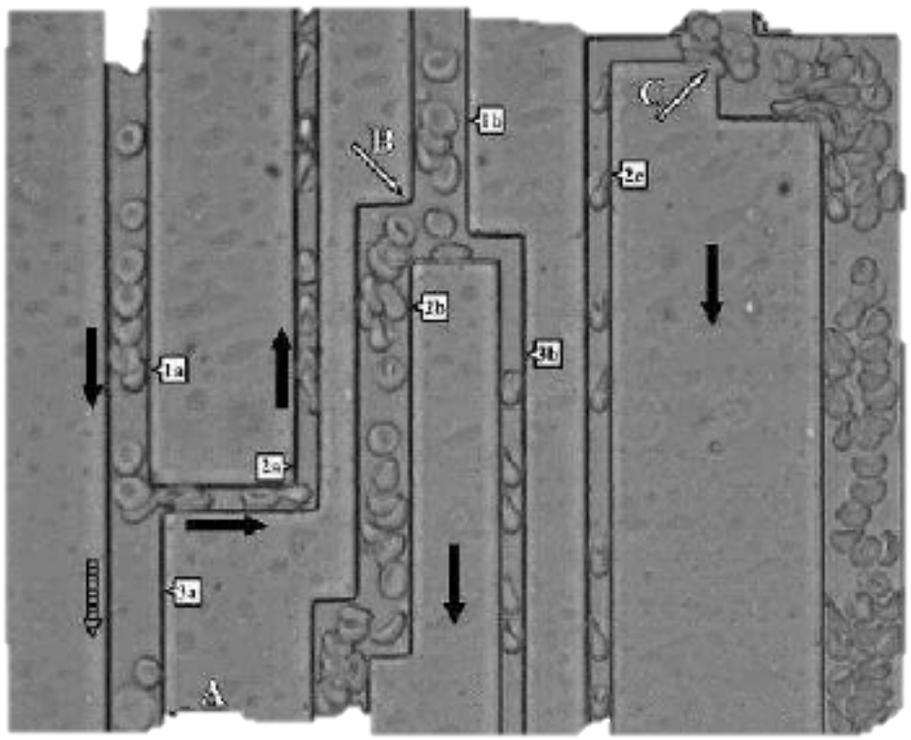
http://www.eatingwithangela.com/EATINGWITHANGELA/assets/Image/EatingWell/WholeWheatGnocchiUncooked.jpg







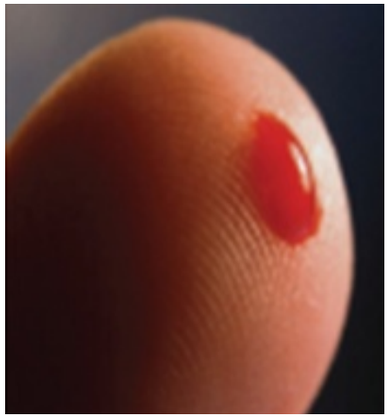


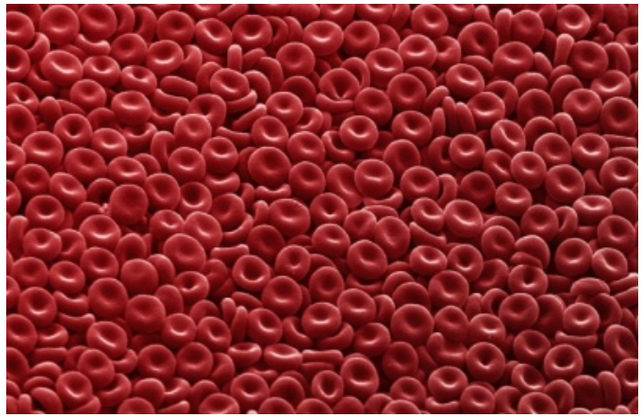


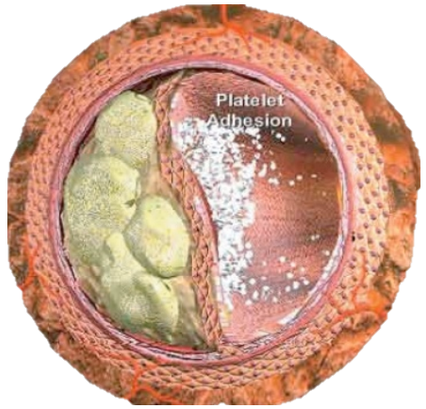
CONTEXT: MOBO

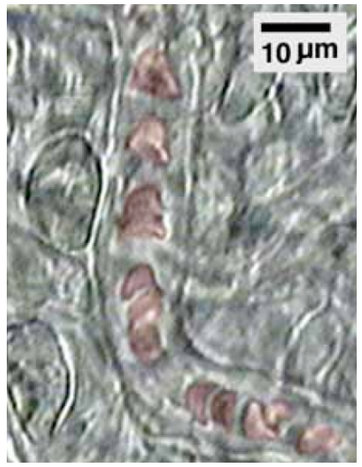
("MOVING BOUNDARIES")

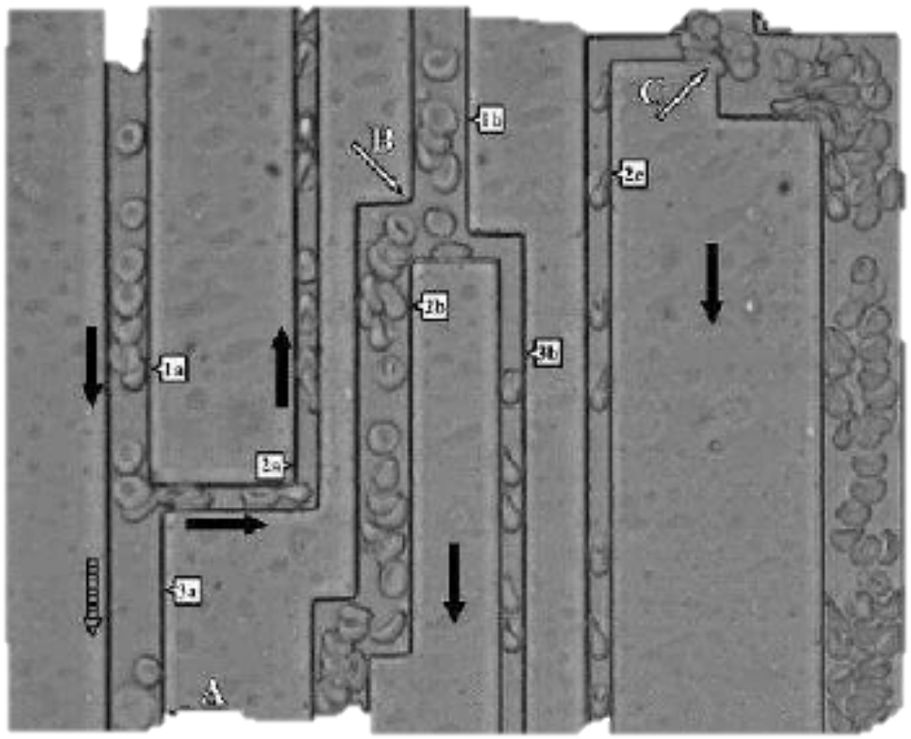
Citation: **A. Rahimian**, I. Lashuk, A. Chandramowlishwaran, D. Malhotra, L. Moon, R. Sampath, A. Shringarpure, S. Veerapaneni, J. Vetter, R. Vuduc, D. Zorin, and **G. Biros**. "Petascale direct numerical simulation of blood flow on 200k cores and heterogeneous architectures." In *Proc. ACM/IEEE Conf. Supercomputing (SC)*, Nov. 2010.
Winner, Gordon Bell Prize. `http://dx.doi.org/10.1109/SC.2010.42`

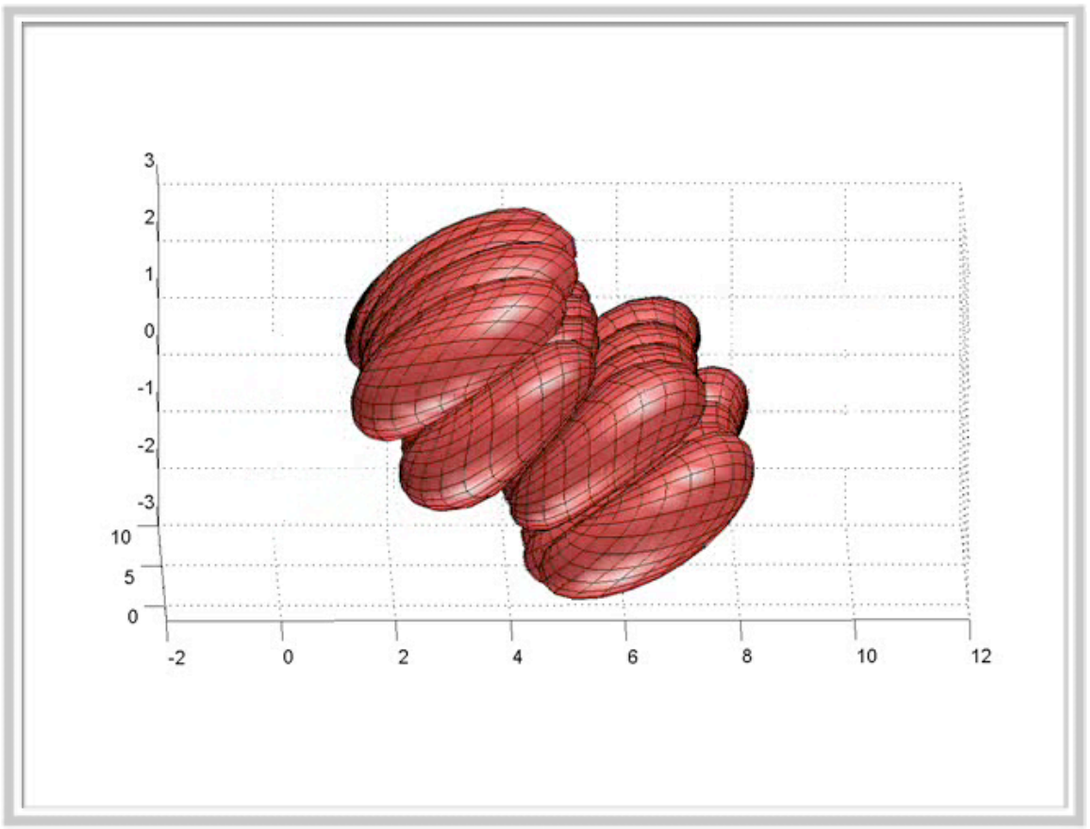












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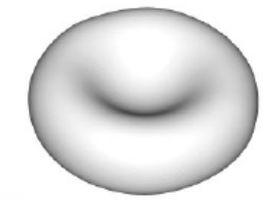
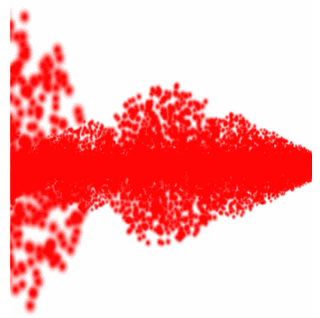
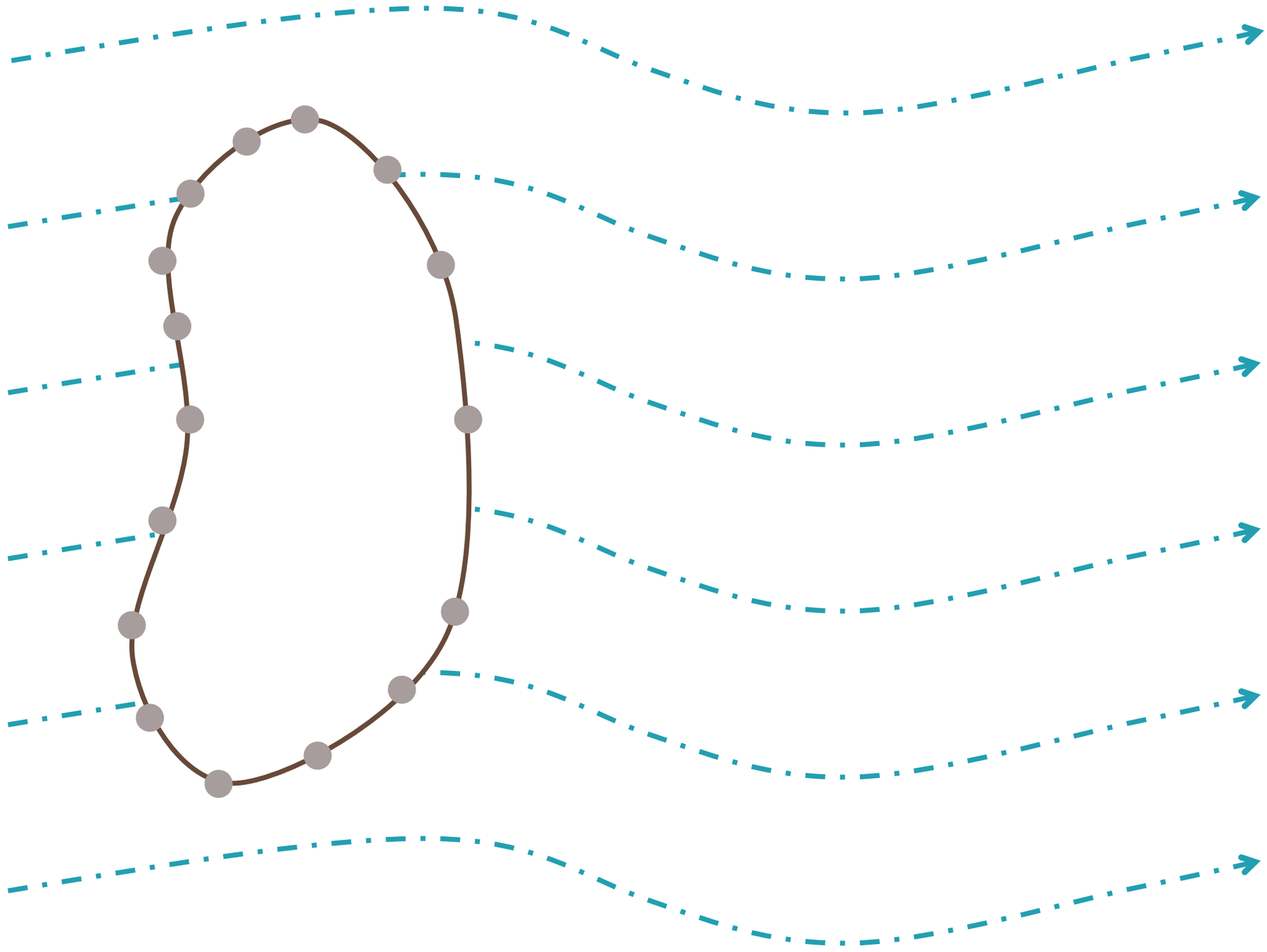
Deformable Red Blood Cells



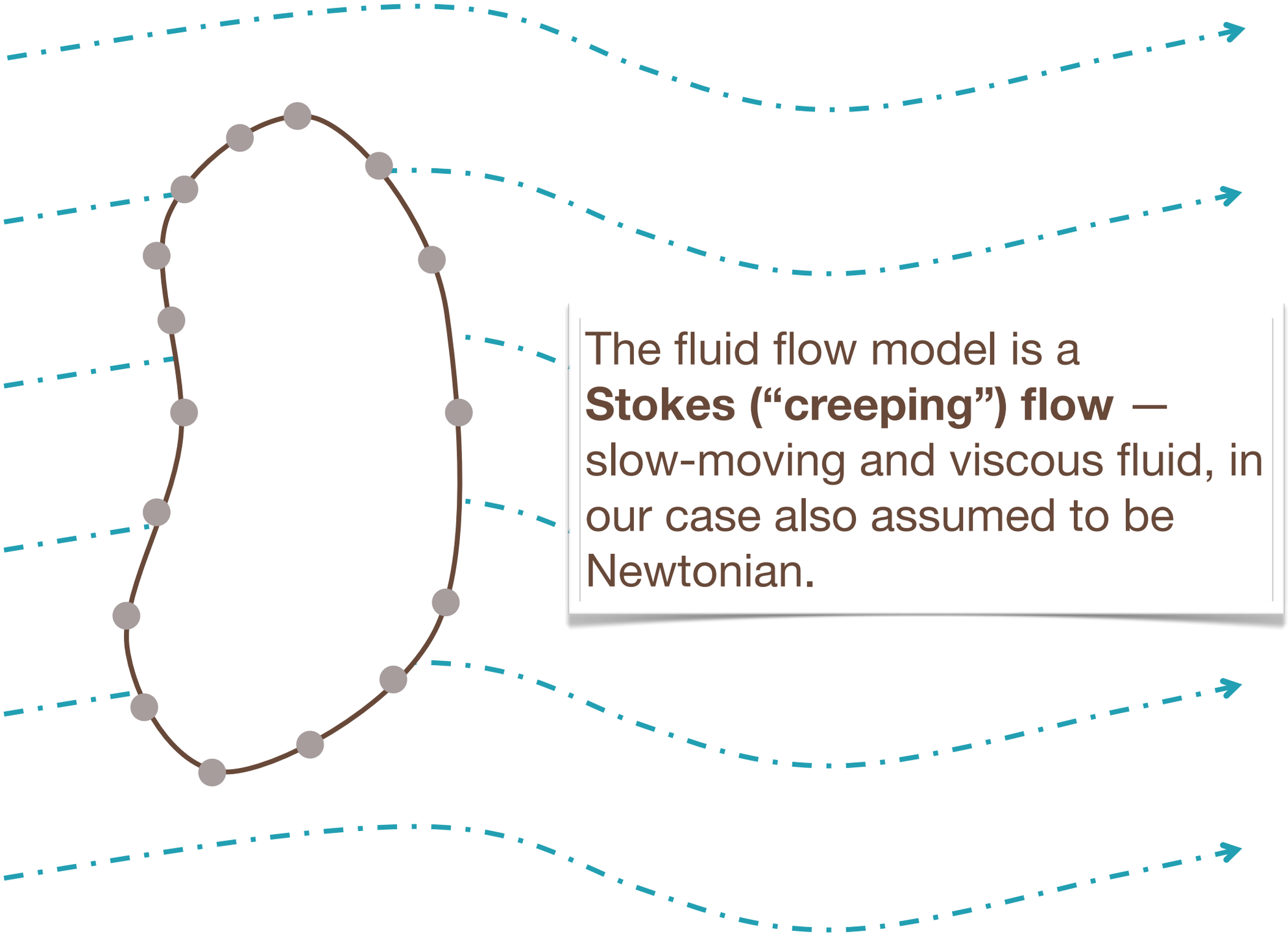


- Prior work with same physical fidelity
  - **1,200 cells**: **Sequential + integral equations**
    Zinchenko et al. (2003)
  - **14,000 cells**: **IBM BG/P + Lattice Boltzmann**
    O(10k) unknowns/cell
    Clausen et al. (2010)
- MoBo: **260 million cells** on **200k cores** (Jaguar @ ORNL)
  - **CPU, GPU + integral equations + implicit AMR**
    O(100) unknowns / cell
  - Key to scaling: Optimal n-body methods based on the
    fast multipole method (FMM) on highly non-uniform domains

- Problem formulation and algorithms

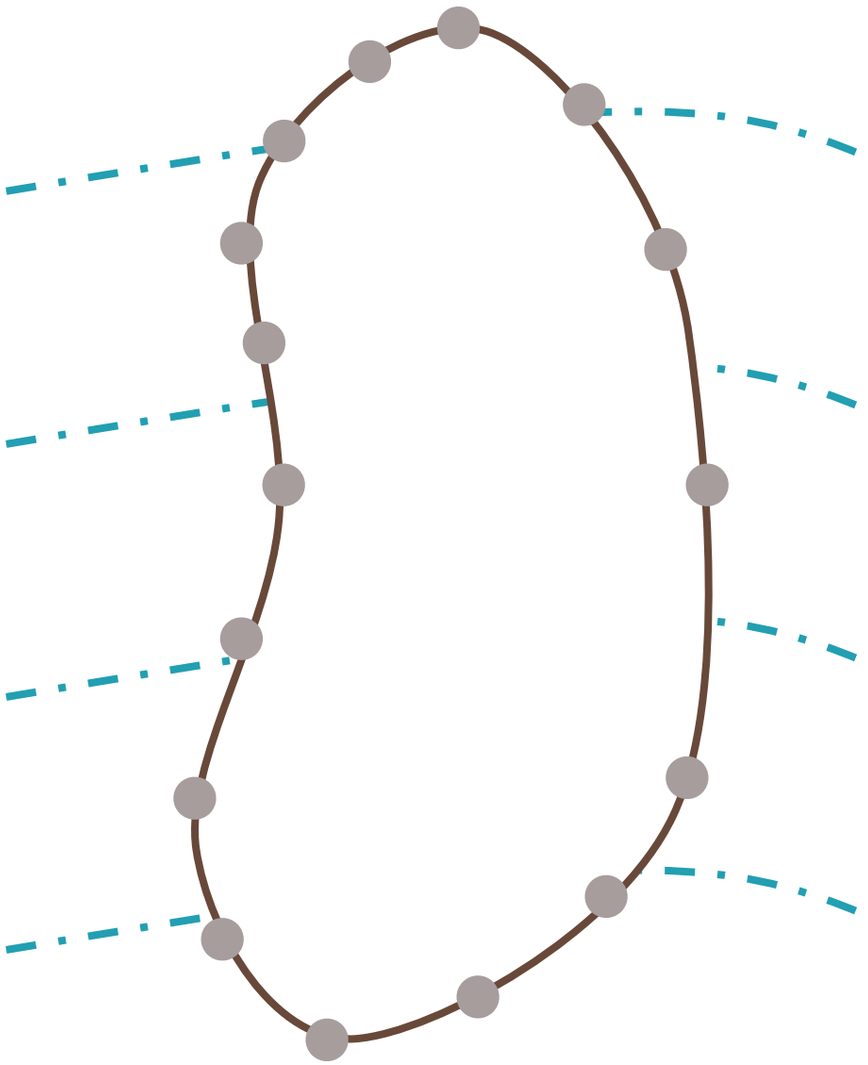


Vesicle flow: Model a red blood cell (RBCs) as fluid-filled deformable and inextensible sac in viscous solution



The fluid flow model is a **Stokes (“creeping”) flow** — slow-moving and viscous fluid, in our case also assumed to be Newtonian.

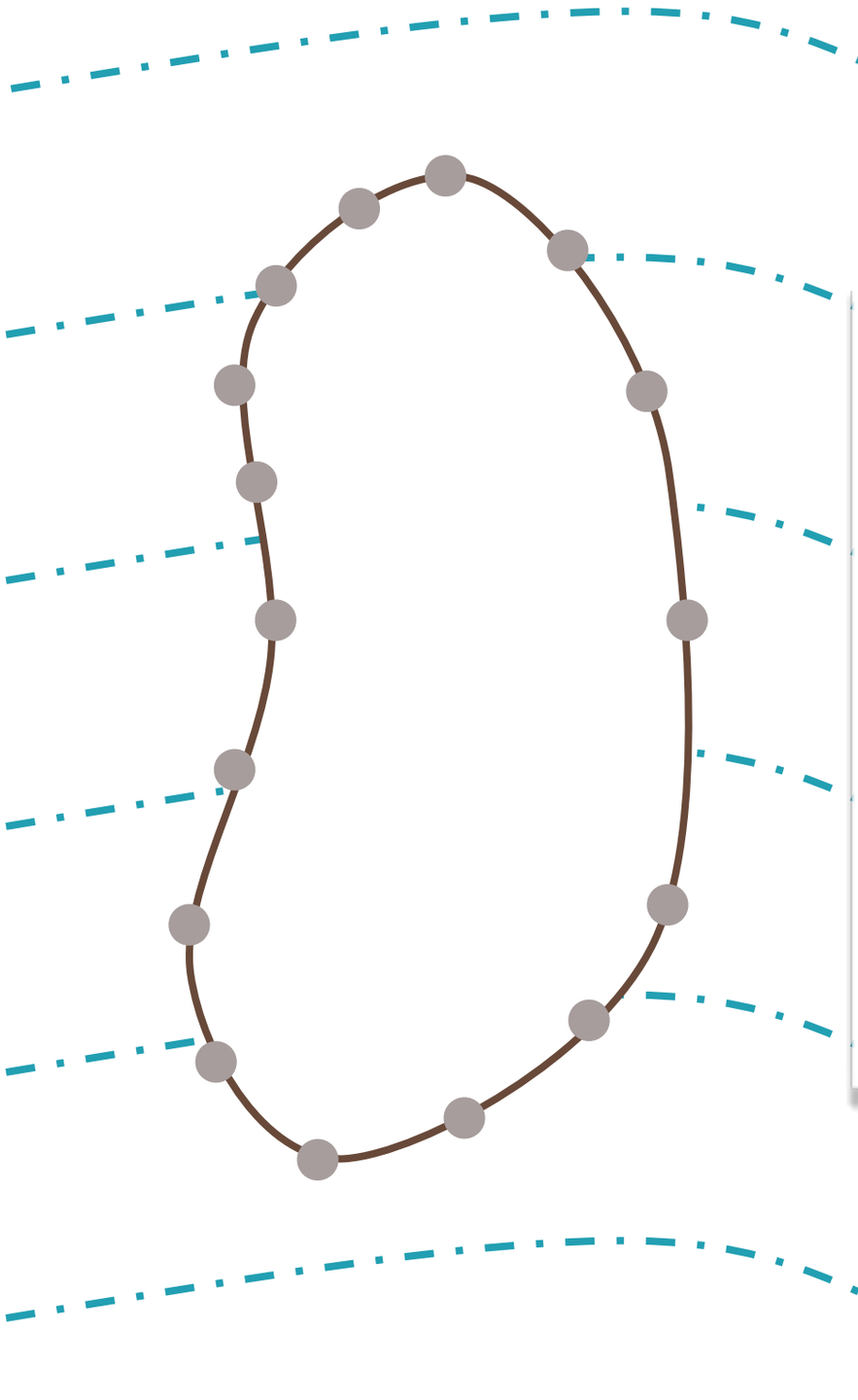
Vesicle flow: Model a red blood cell (RBCs) as fluid-filled deformable and inextensible sac in viscous solution



The numerical method is based on a **boundary integral formulation**, in which the fluid is represented implicitly and we need only discretize the cell boundary.[1]

[1] In contrast to Lattice Boltzman or finite-element methods, in which we discretize the entire domain.

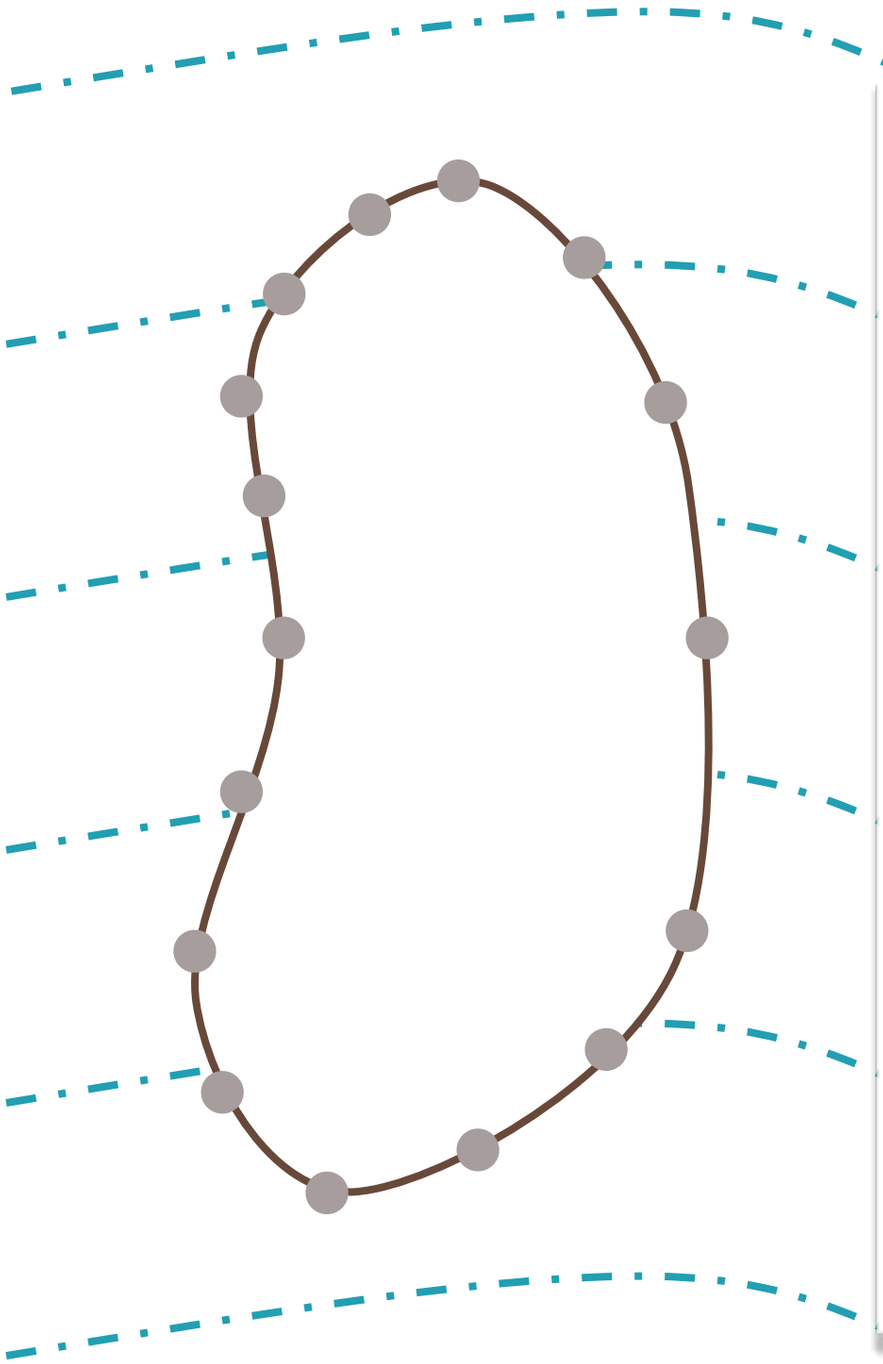
Vesicle flow: Model a red blood cell (RBCs) as fluid-filled deformable and inextensible sac in viscous solution



Challenges in implementing boundary integral methods:

- Stiffness, due to high-order derivatives required to accurately capture RBC deformations
- Efficient evaluation of long-range interactions

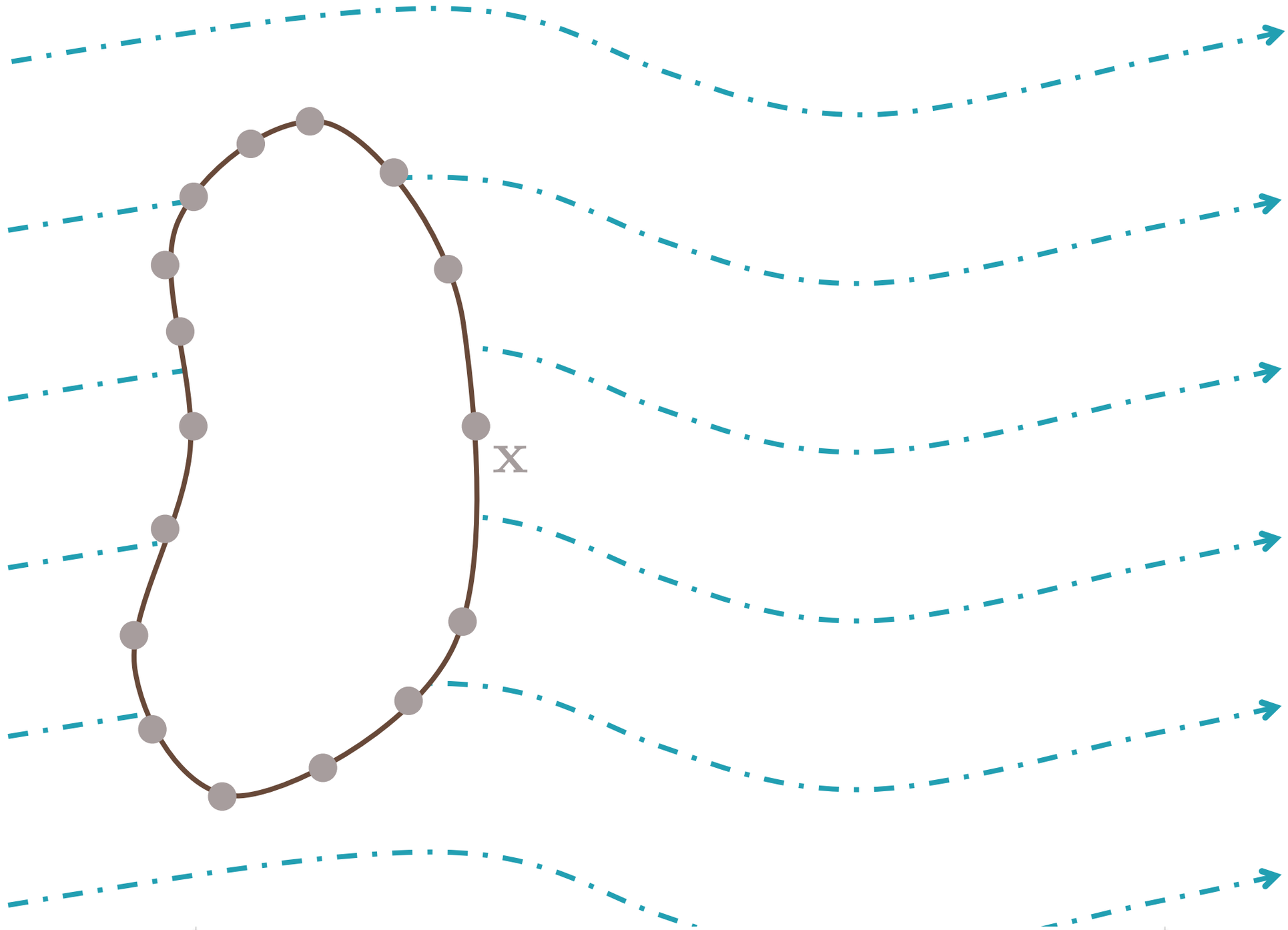
Vesicle flow: Model a red blood cell (RBCs) as fluid-filled deformable and inextensible sac in viscous solution



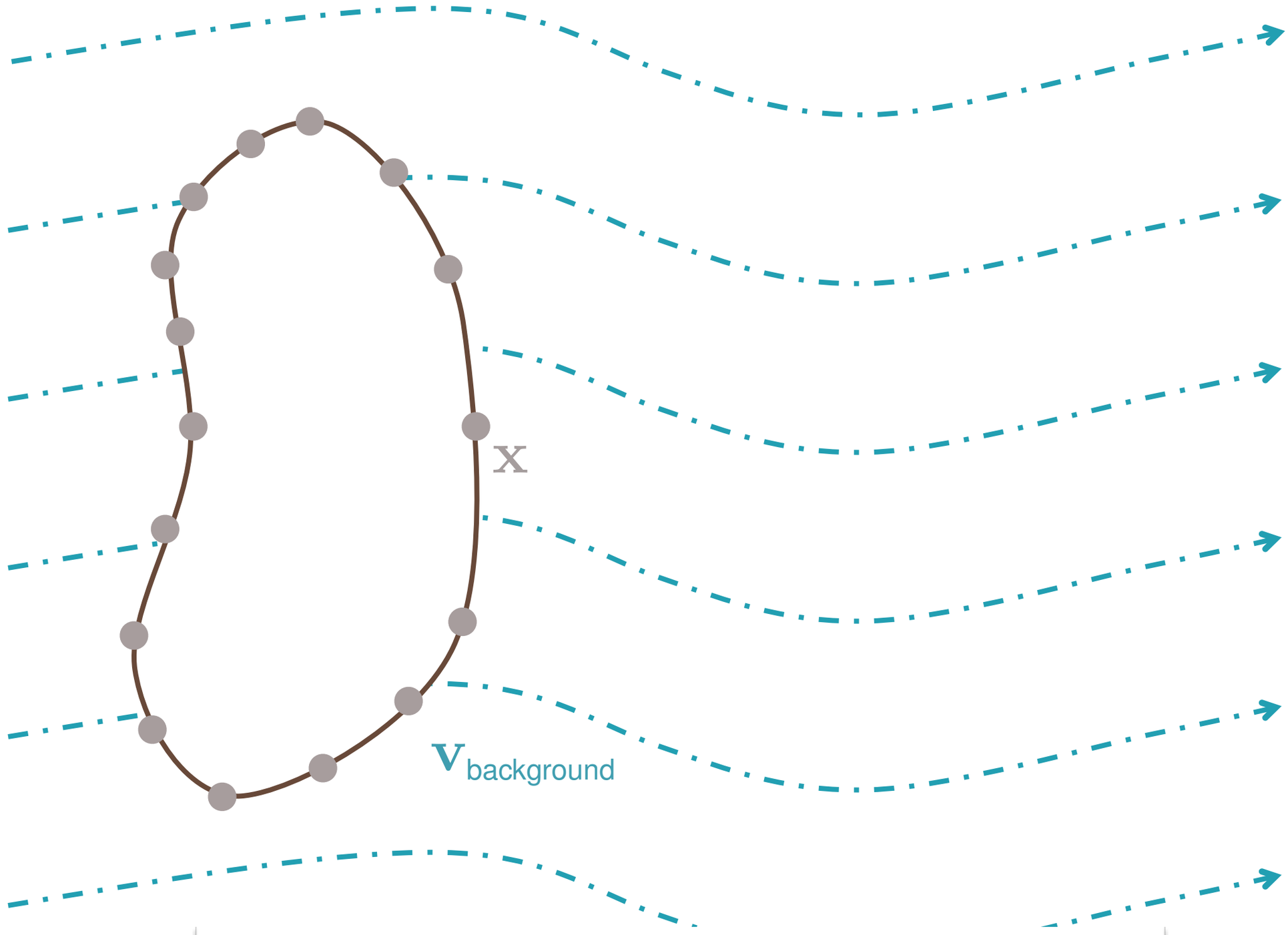
Features of our approach:

- Represent RBC in a **spherical harmonics** basis, which permits accurate high-order derivative computations
- Efficient evaluation of long-range interactions via **FMM**
- Time-stepping with a **multistep, semi-implicit** method that is, at least empirically, unconditionally stable

Vesicle flow: Model a red blood cell (RBCs) as fluid-filled deformable and inextensible sac in viscous solution



$$\frac{d\mathbf{x}}{dt} = \mathbf{v}_{\text{background}}(\mathbf{x}) + \mathbf{v}_{\text{interaction}}(\mathbf{x})$$



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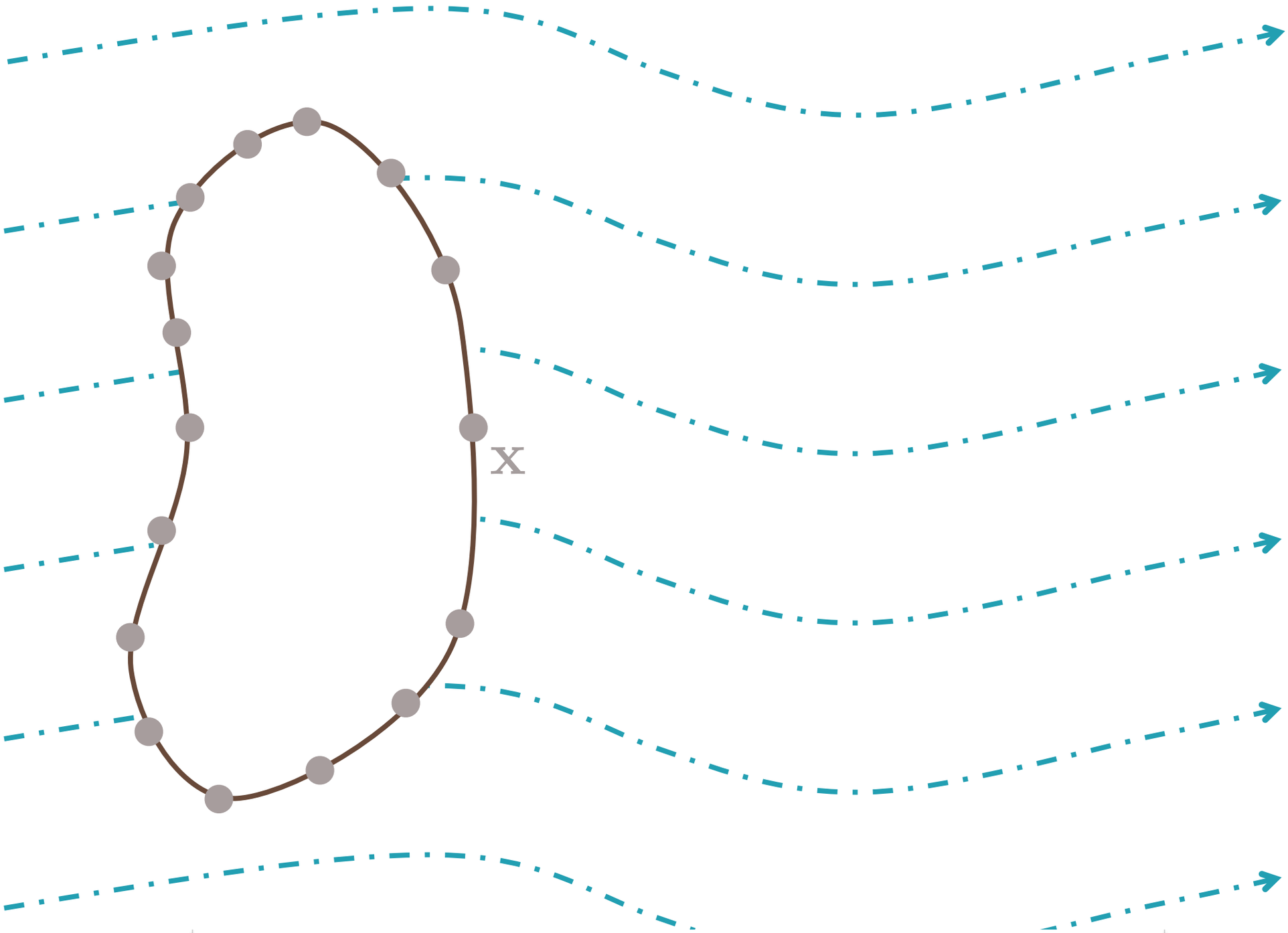
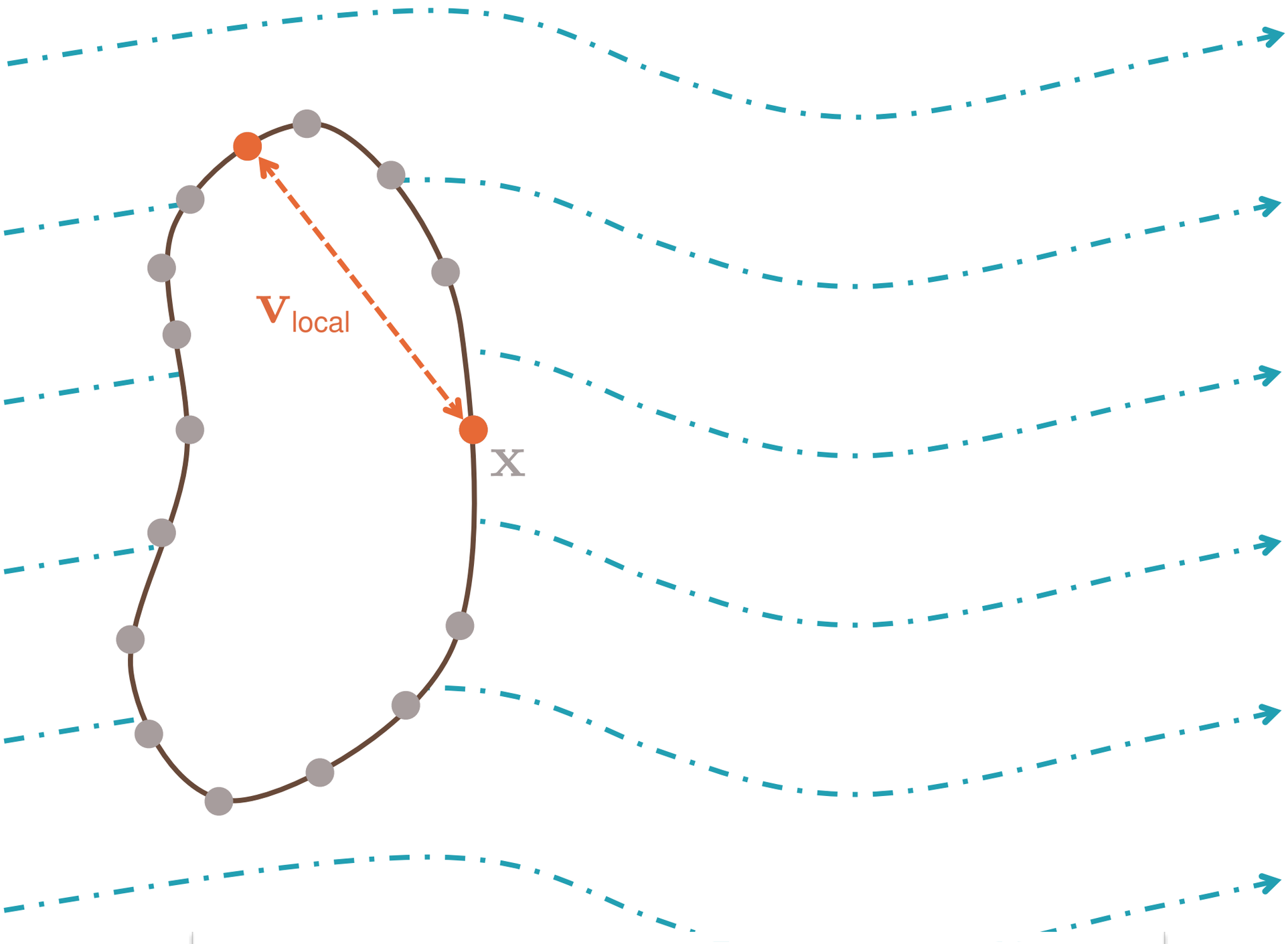


$$\mathbf{v}_{\text{interaction}}(\mathbf{x}) = \mathbf{v}_{\text{local}}(\mathbf{x}) + \mathbf{v}_{\text{global}}(\mathbf{x})$$



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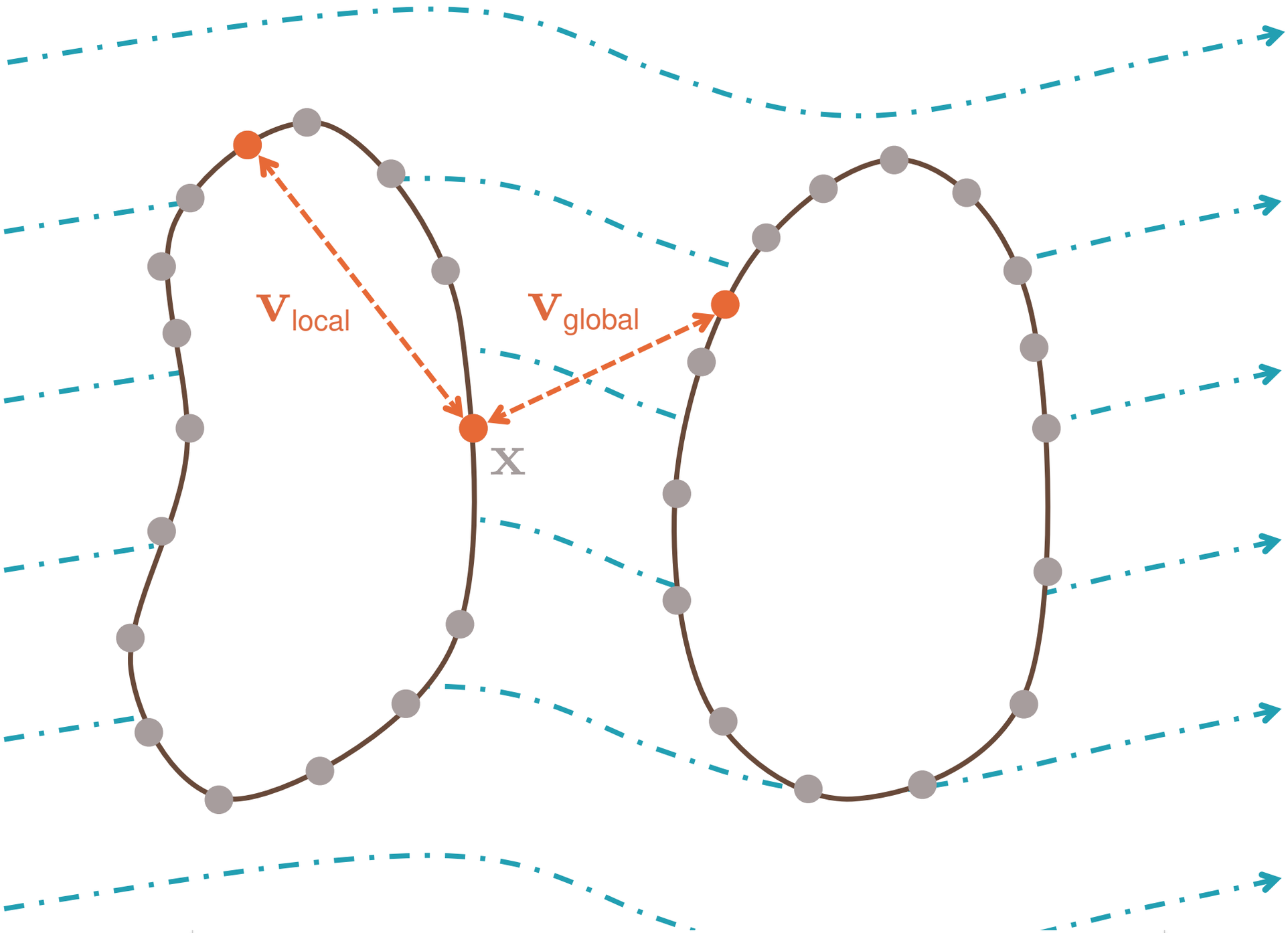

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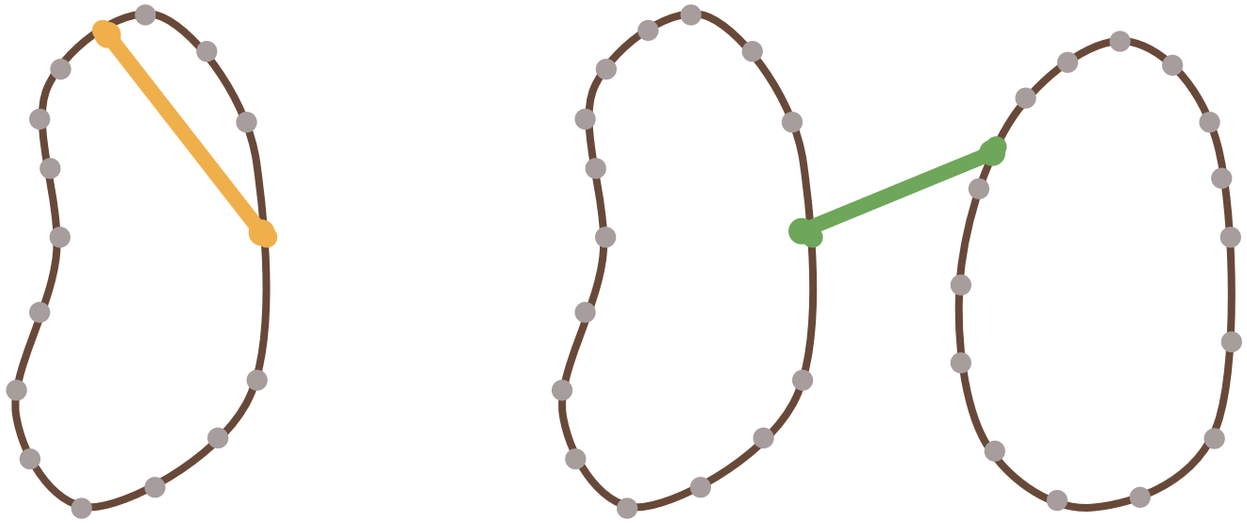
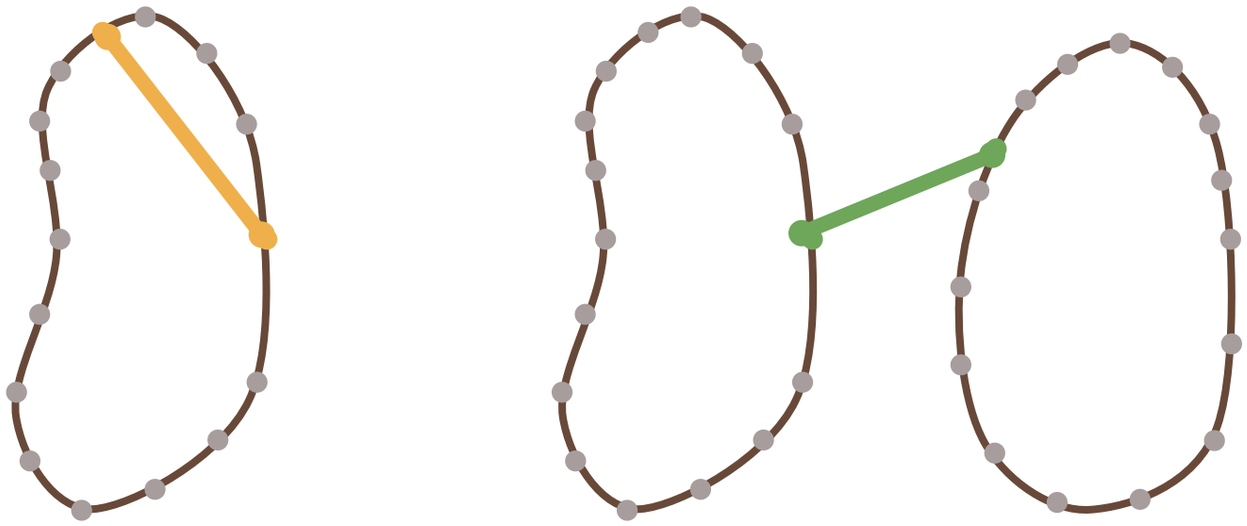
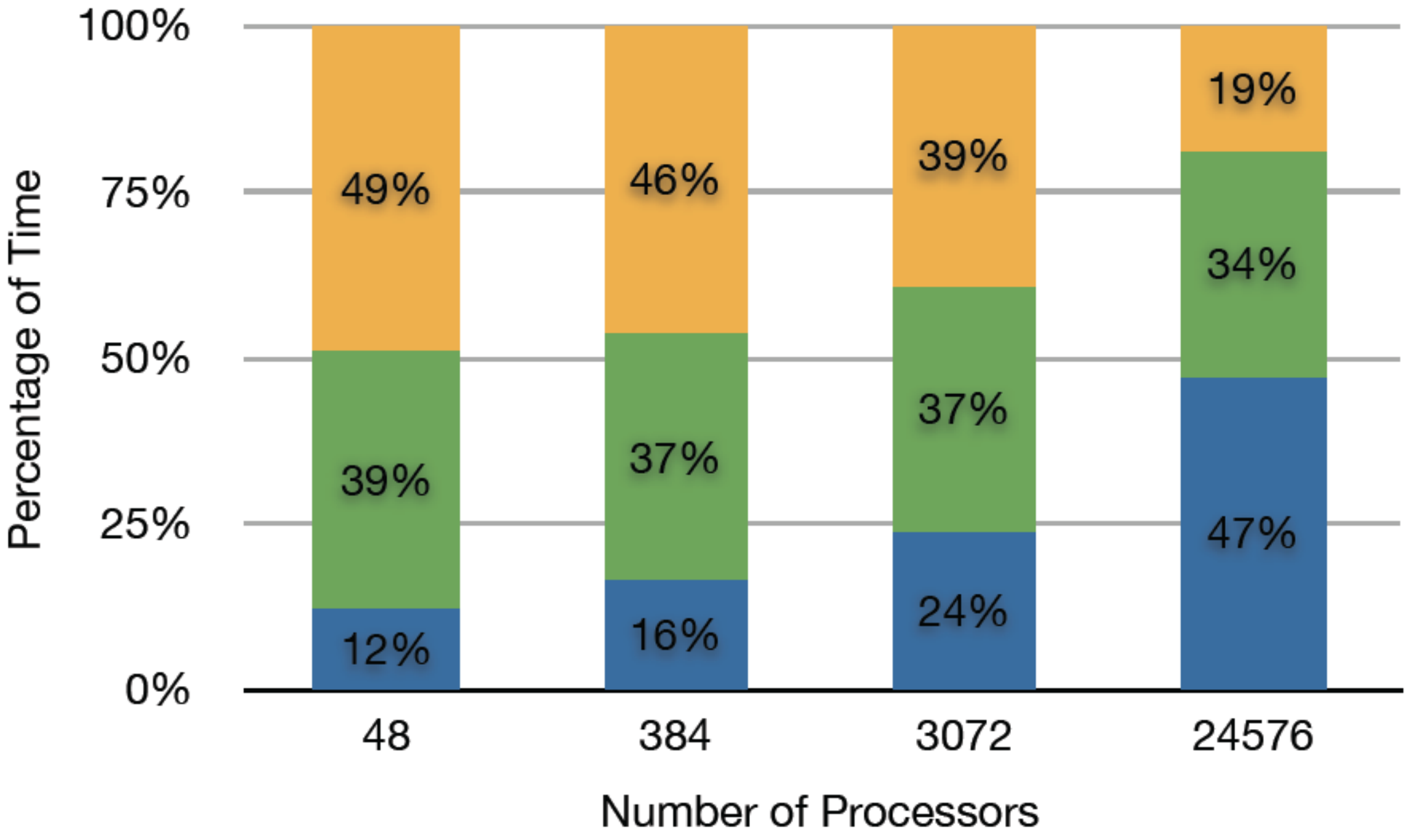
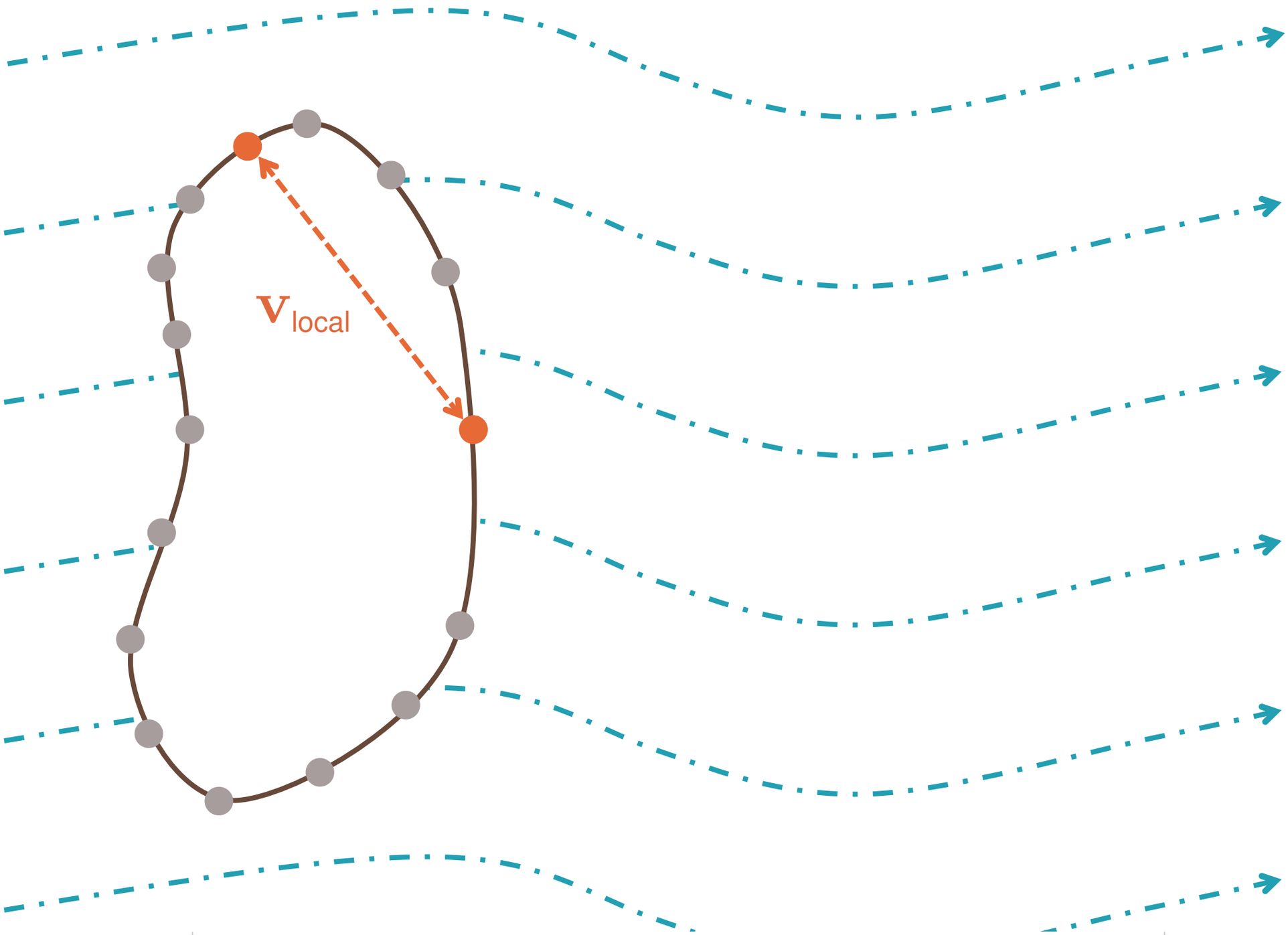





100%
75%
50%
25%
0%
Percentage of Time
49%
39%
12%
46%
37%
16%
39%
37%
24%
19%
34%
47%
48
384
3072
24576
Number of Processors



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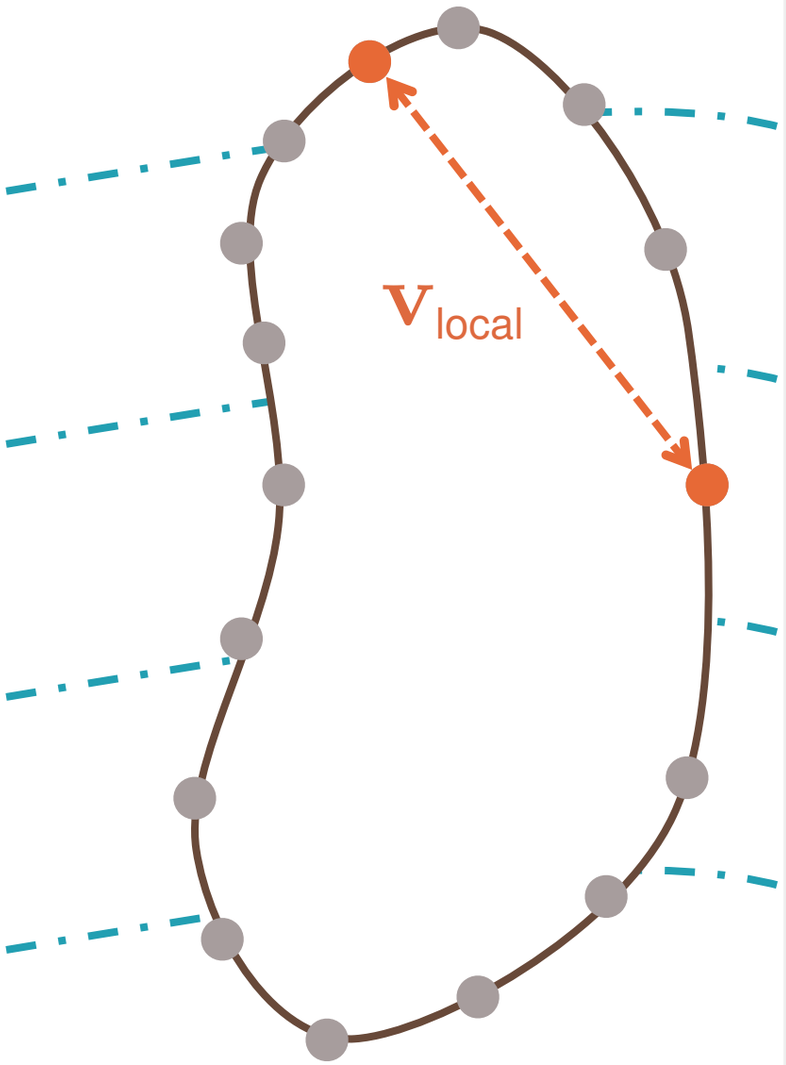


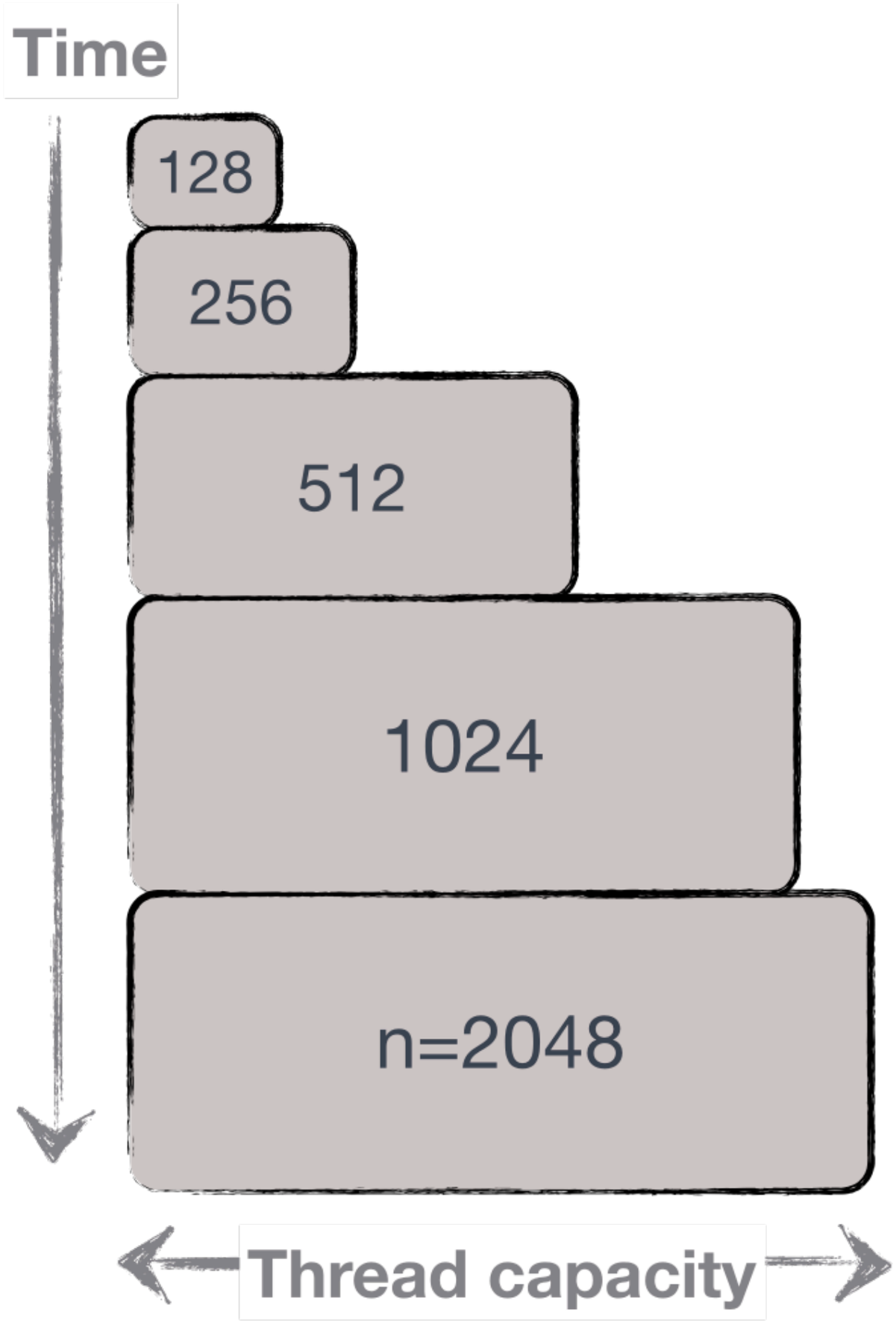
Intra-cell forces computation:

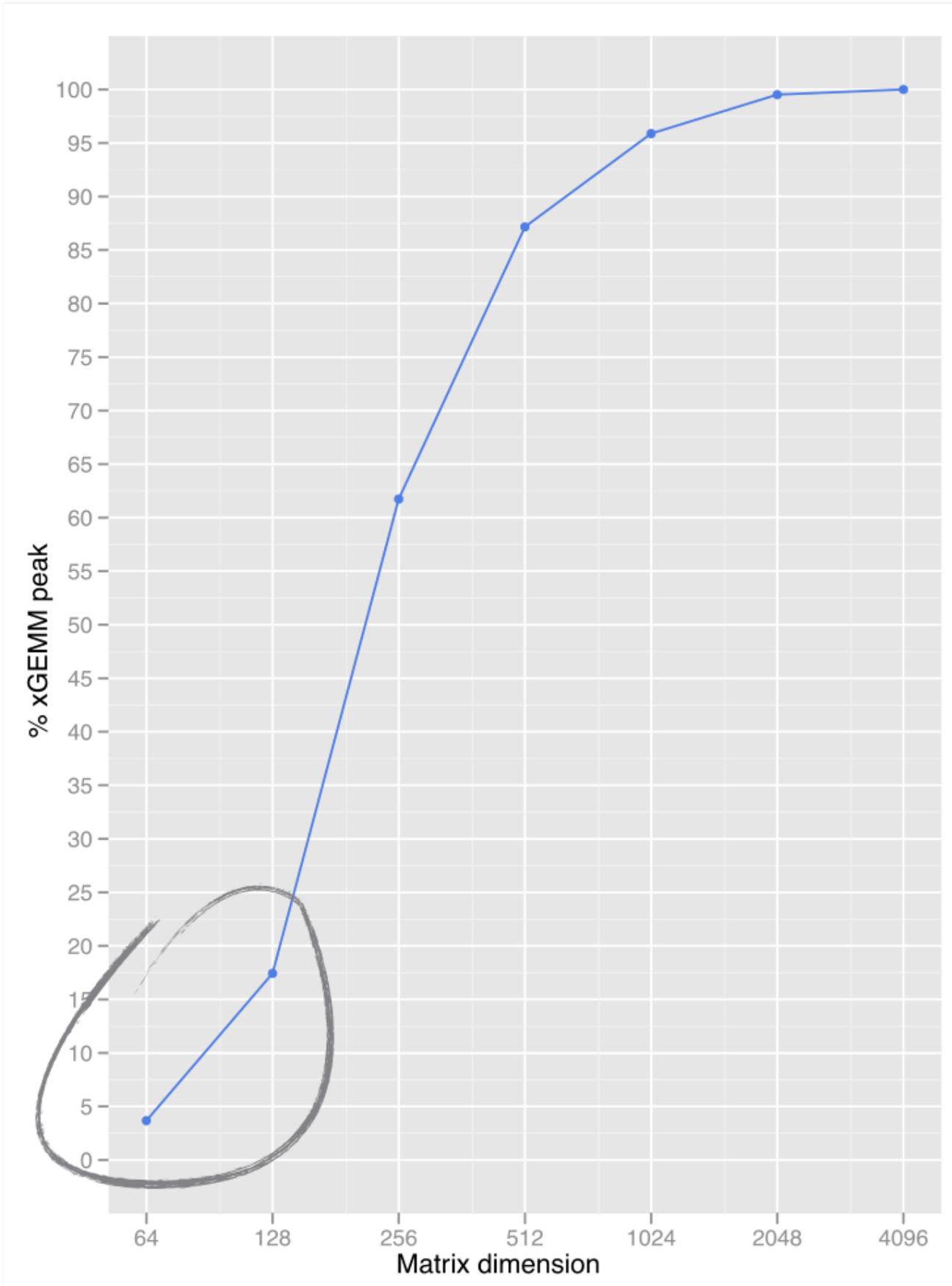
- Spherical harmonics (Legendre & Fourier transforms)
- Singular quadratures
- Derivatives
- Surface remeshing
- Semi-implicit solver (BiCGStab)

Pleasingly parallel over RBCs.

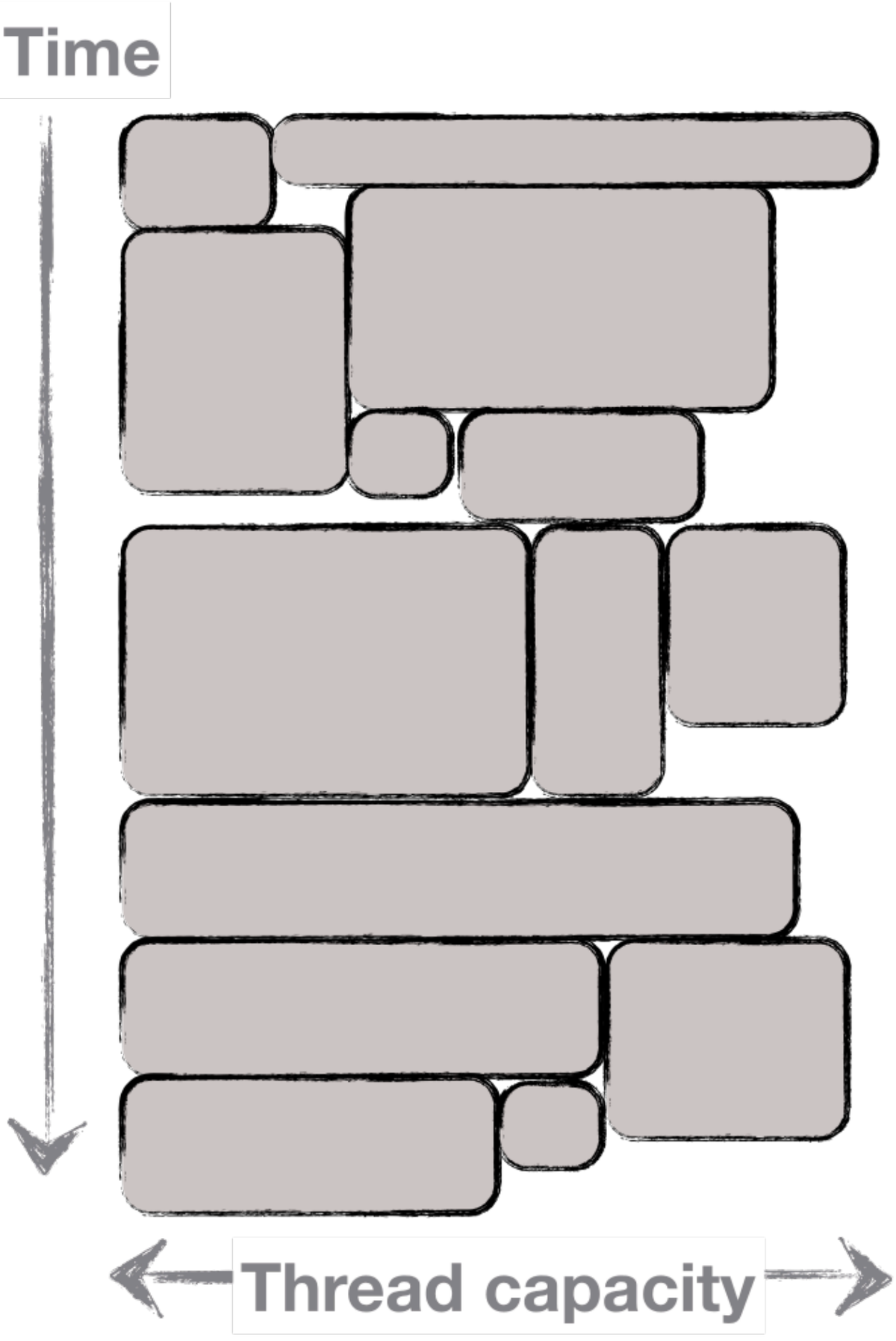
Time dominated by ~ many small matrix multiplies.

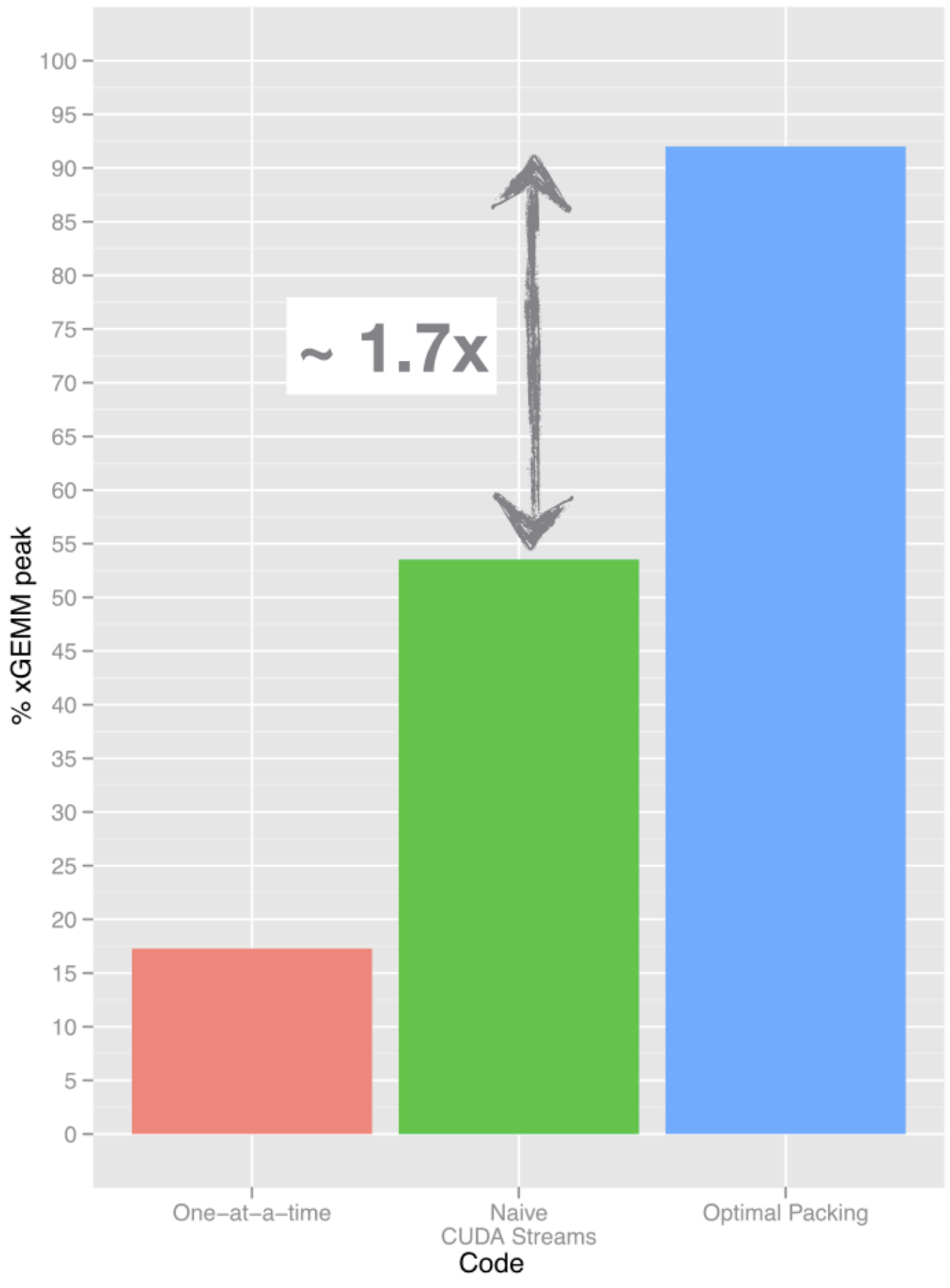
$$\mathbf{v}_{\text{interaction}}(\mathbf{x}) = \mathbf{v}_{\text{local}}(\mathbf{x}) + \mathbf{v}_{\text{global}}(\mathbf{x})$$


Time
128
256
512
1024
n=2048
Thread capacity

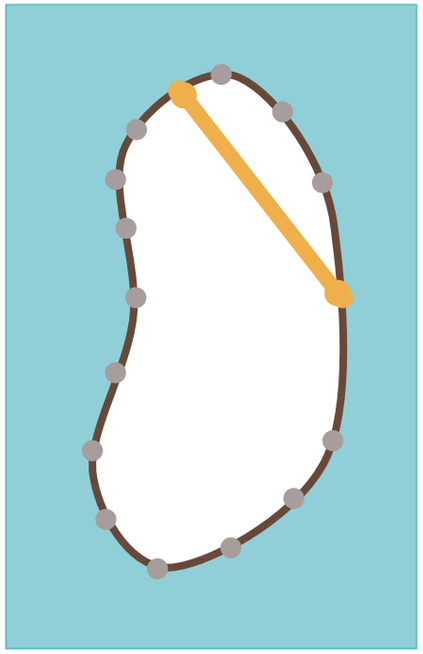

100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
% xGEMM peak
64
128
256
512
1024
2048
4096
Matrix dimension

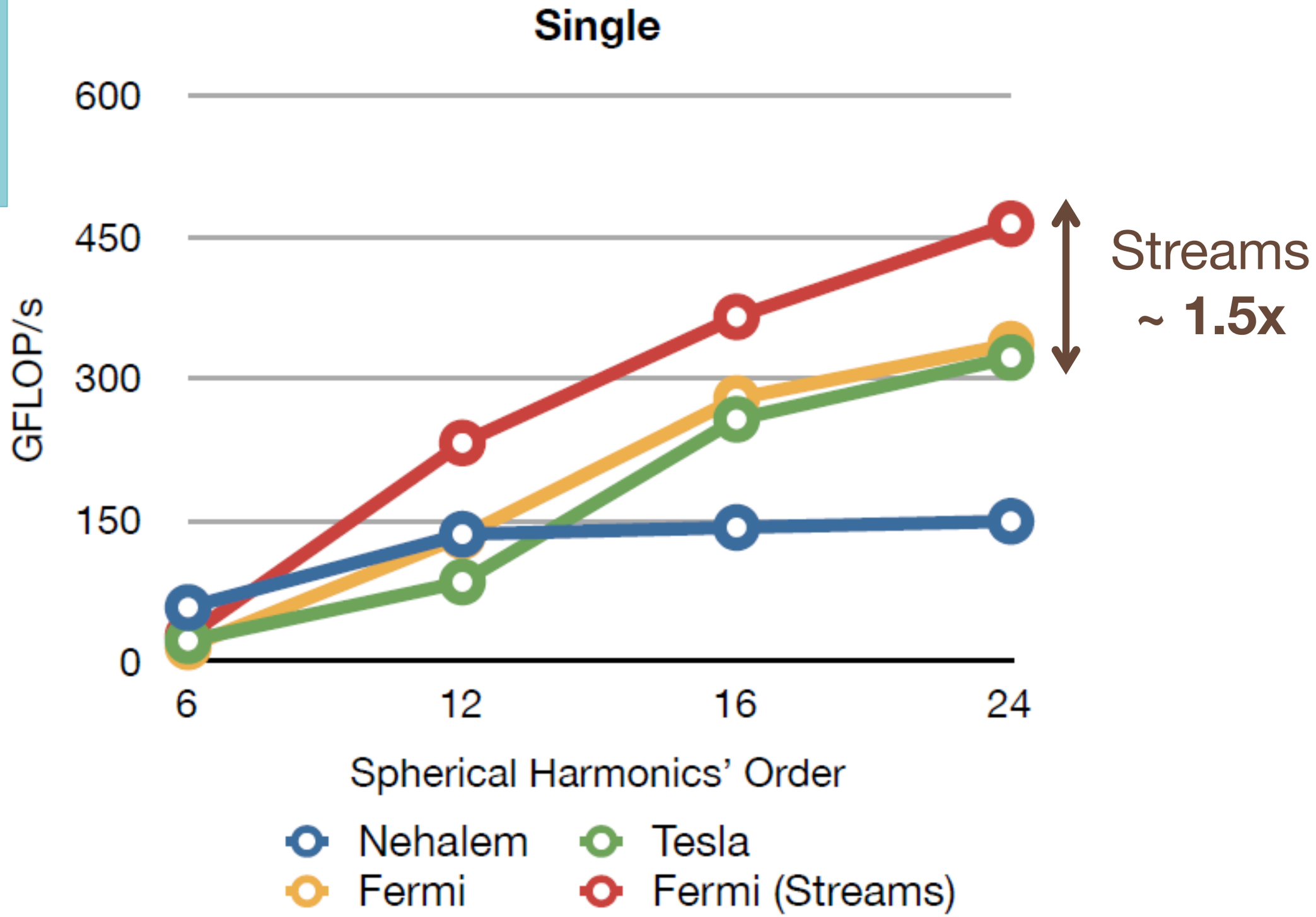
Given a sequence of “small” independent kernel invocations, we use the **CUDA Streams interface** to fill capacity.



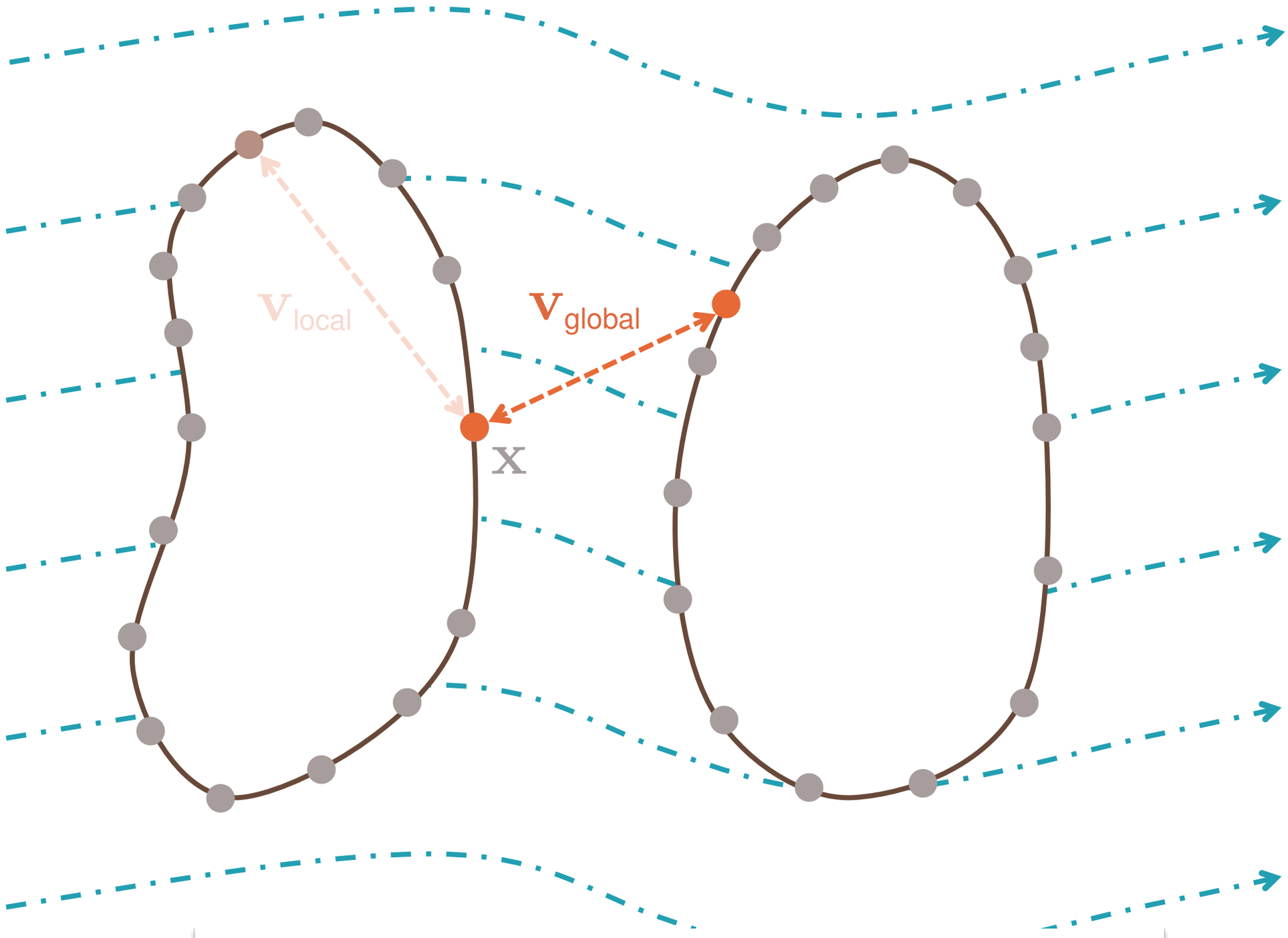


Kent Czechowski <kentcz@gatech.edu>

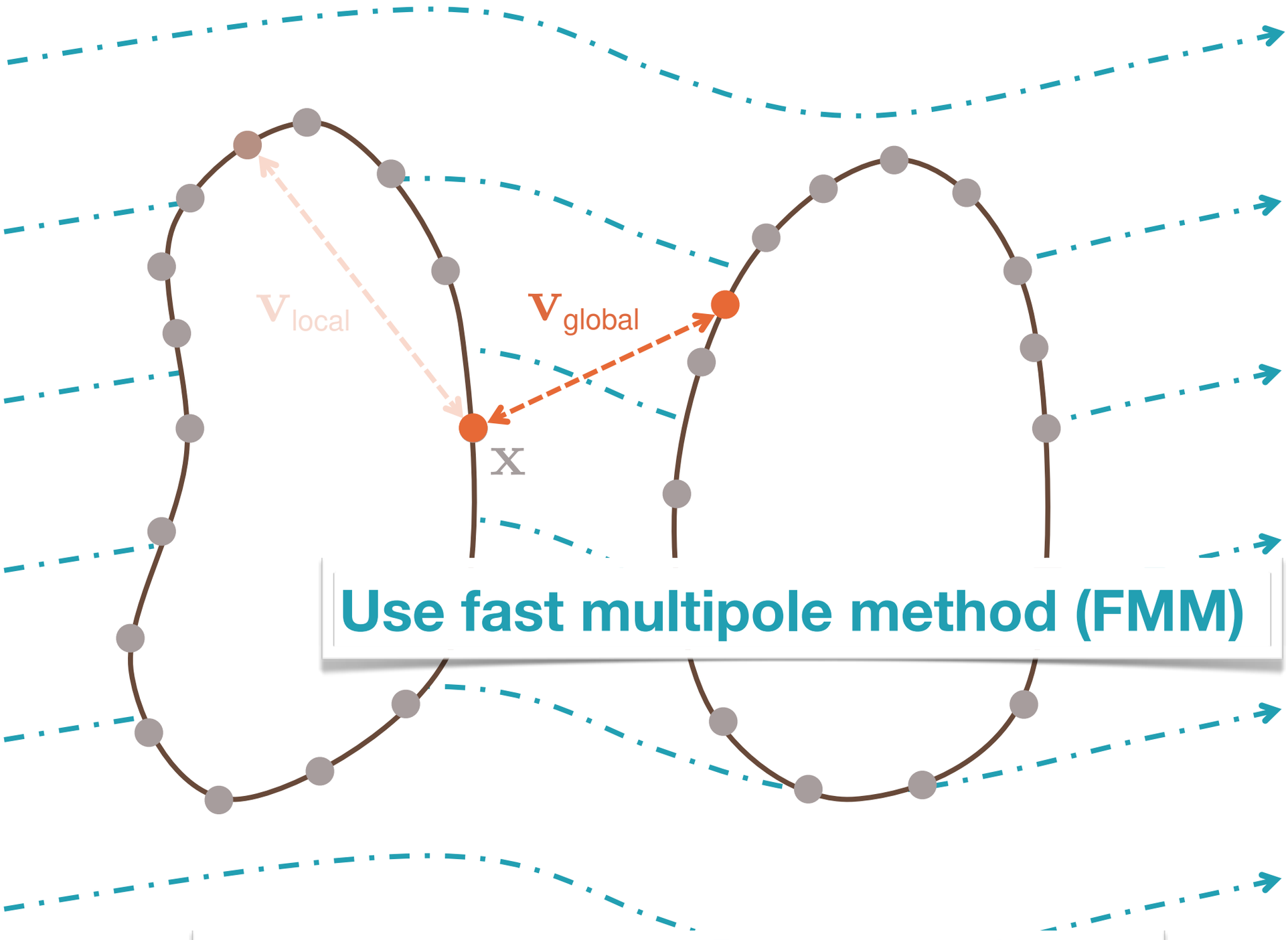




Peng Wang & Steve Parker @ NVIDIA



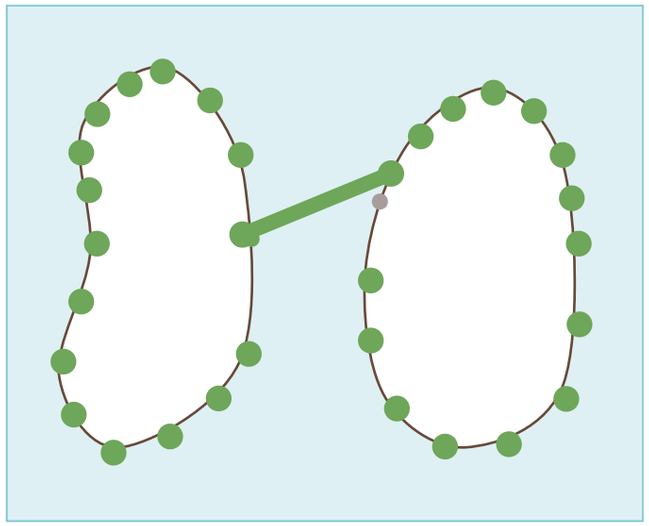
$$\mathbf{v}_{\text{interaction}}(\mathbf{x}) = \mathbf{v}_{\text{local}}(\mathbf{x}) + \mathbf{v}_{\text{global}}(\mathbf{x})$$



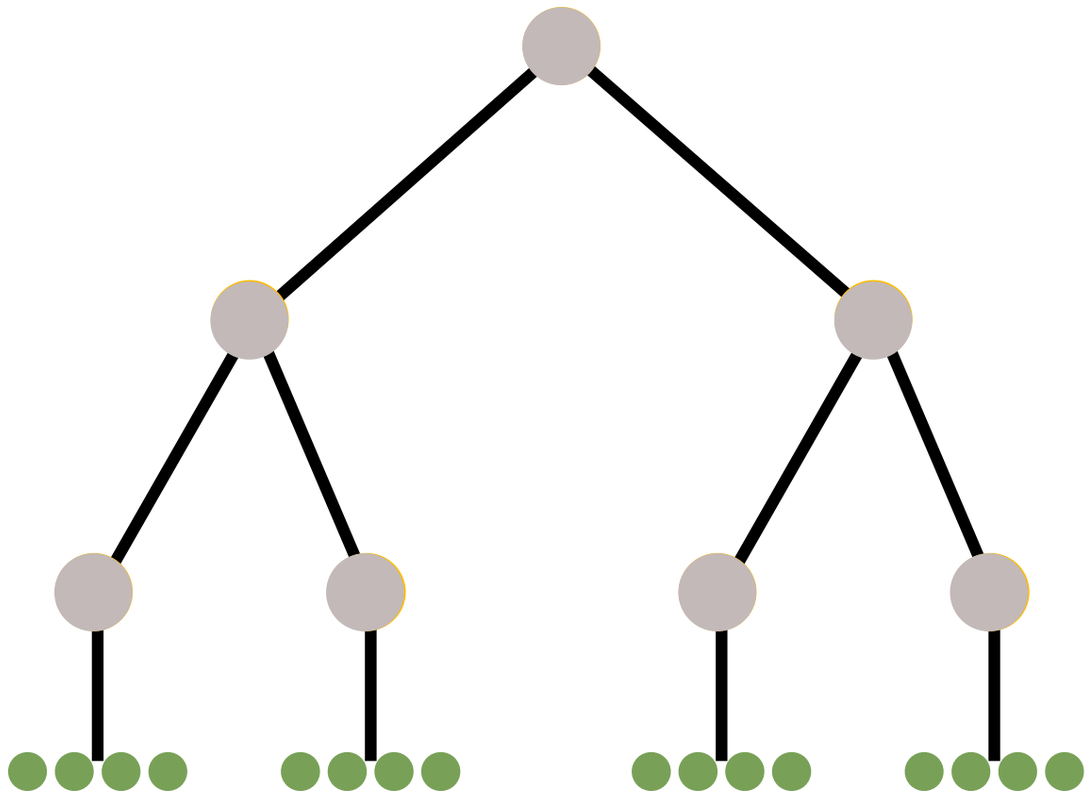
Use fast multipole method (FMM)

$$\mathbf{v}_{\text{interaction}}(\mathbf{x}) = \mathbf{v}_{\text{local}}(\mathbf{x}) + \mathbf{v}_{\text{global}}(\mathbf{x})$$

FMM

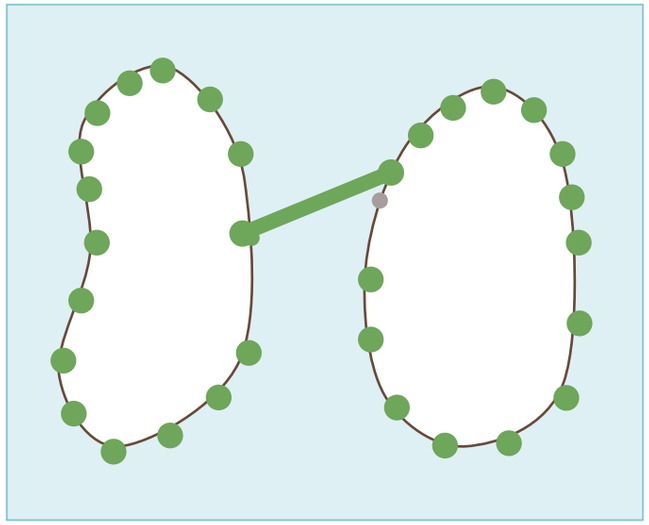


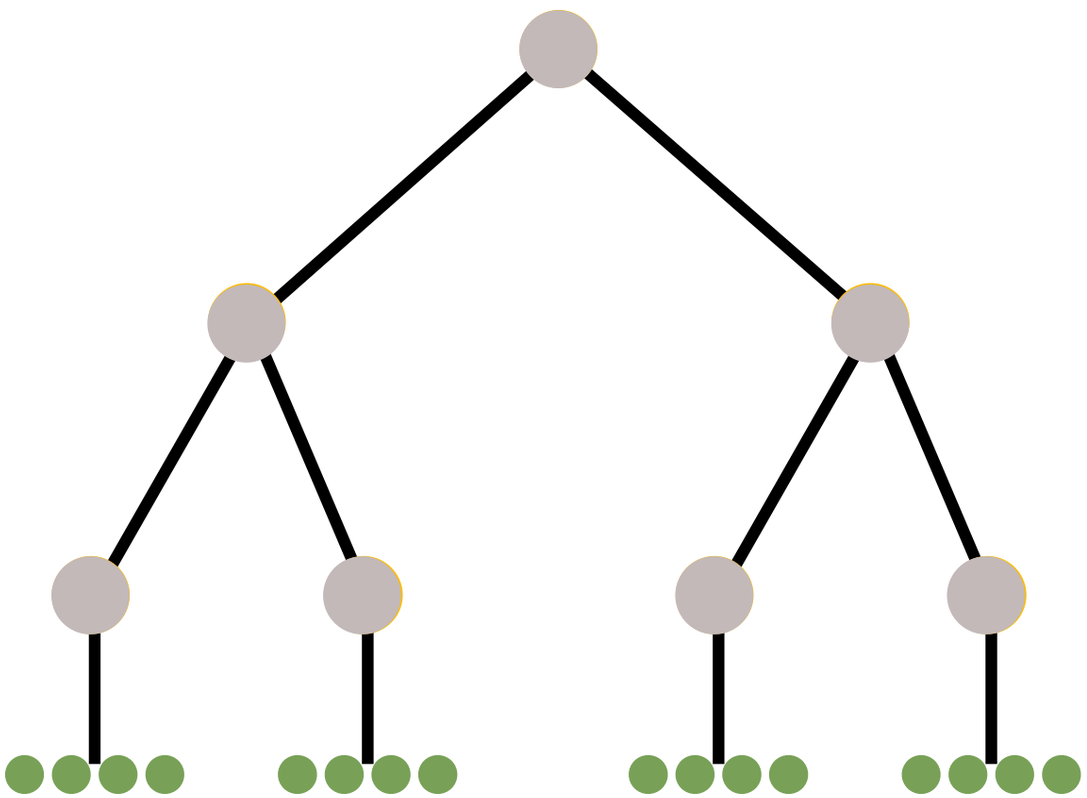
- Need to evaluate all-pairwise interactions among green points: **$O(n^2)$**



- FMM instead computes in **O(n)** time, with an approximation guarantee, using a tree (**n log n** to build)

Distributed Memory Algorithm





- We use a *kernel-independent* variant, but the structure and parallelization are same as classical case [Warren & Salmon (1993)]
- "Control" adaptivity using 2:1 balancing [Sampath et al. (2008)]

Summary: Basic Algorithm

- Given: n RBCs, where the k-th RBC is represented by the set γ_k of its surface points
- Loop over time steps (multistep):
  - **Parallel-for $k \leftarrow 1{:}n$, compute $v_{\text{local}}(x)$ for all x in γ_k**
  - **Compute $v_{\text{global}}(x)$ using the FMM**
  - Evaluate $v_{\text{background}}(x)$ analytically
  - Update positions (semi-implicit)
  - Periodically load re-balance (repartition)

Complexity Estimates

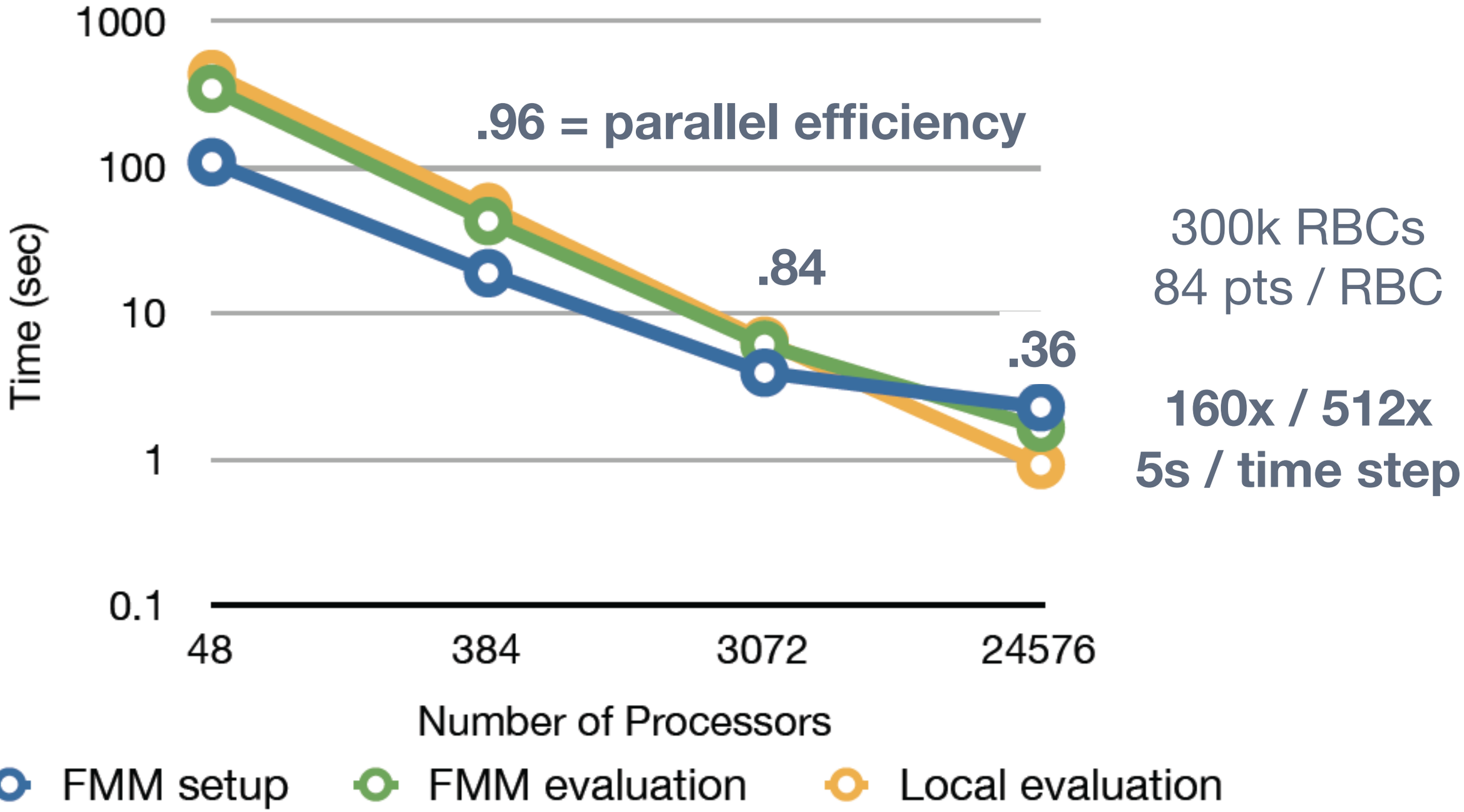
$\mathbf{v}_{\text{local}}$: $$\mathcal{O}\left(\eta^{\frac{3}{2}} \cdot \frac{n}{p}\right)$$

$\eta =$ points / cell, $n =$ total points

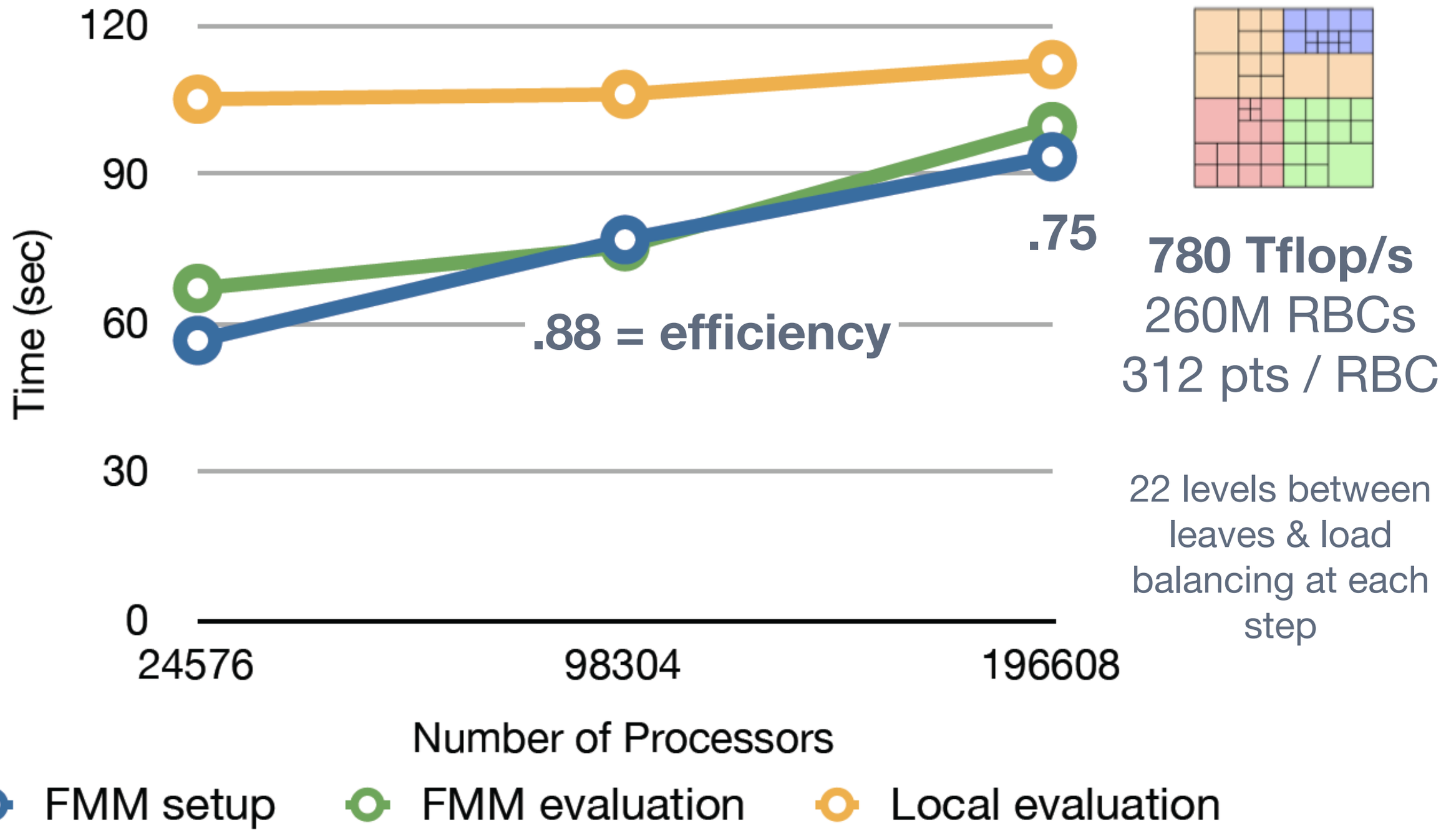
$\mathbf{v}_{\text{global}}$, build tree : $$\mathcal{O}\left(\frac{n}{p}\log\frac{n}{p} + \sqrt{p}\left(\frac{n}{p}\right)^{\frac{2}{3}} + p\log^2 p\right)$$

$\mathbf{v}_{\text{global}}$, evaluation : $$\mathcal{O}\left(\frac{n}{p} + \sqrt{p}\left(\frac{n}{p}\right)^{\frac{2}{3}}\right)$$

STRONG SCALING: JAGUAR



Weak Scaling: Jaguar

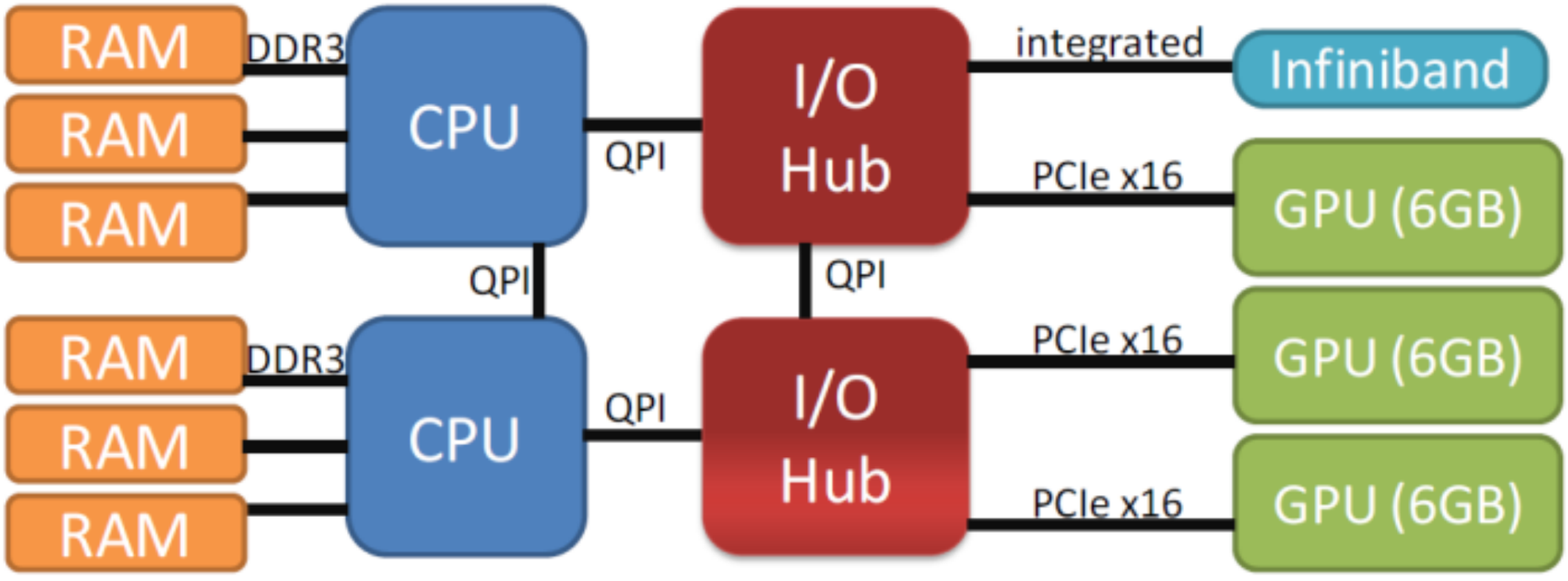


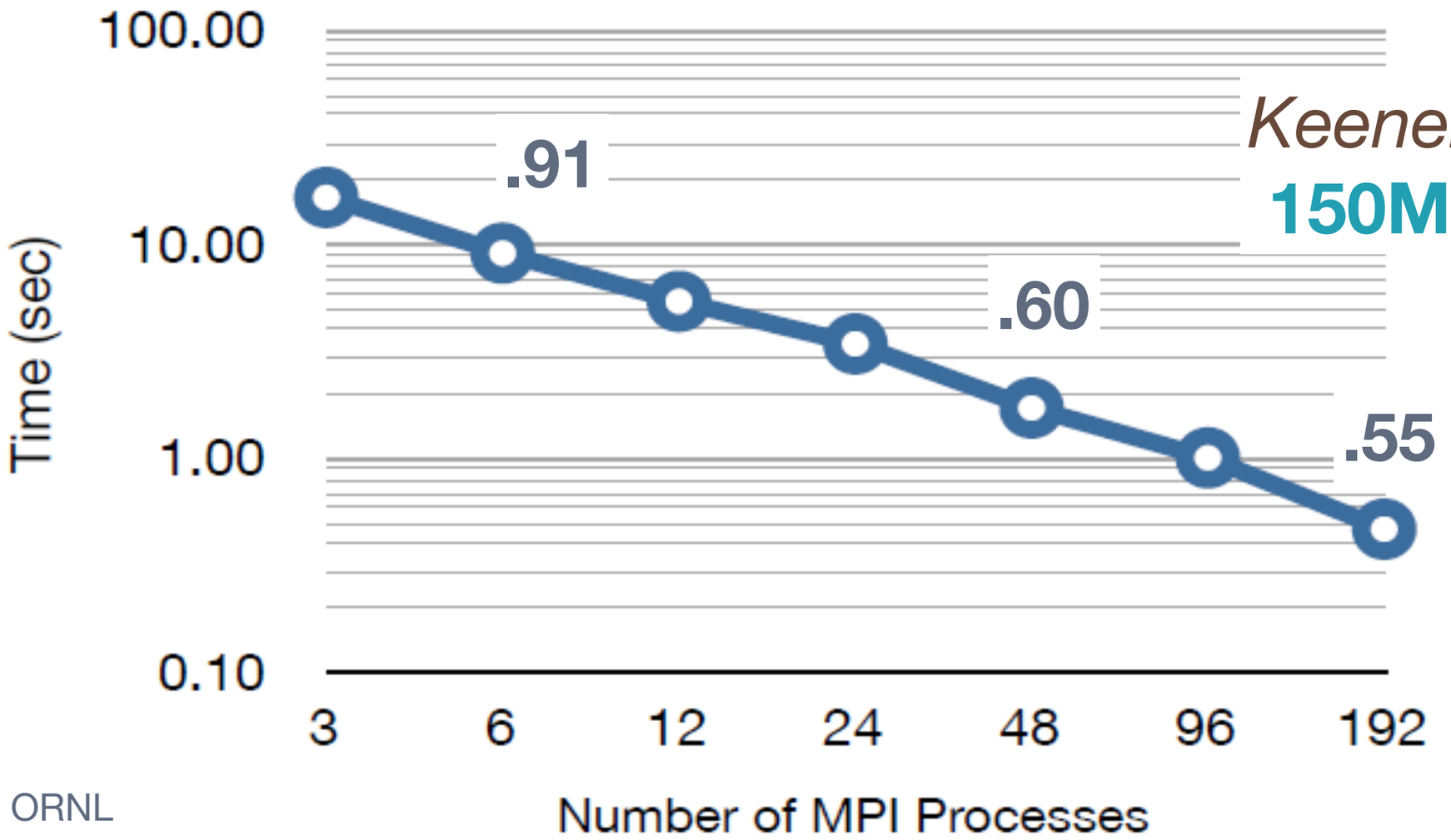
780 Tflop/s

260M RBCs

312 pts / RBC

22 levels between leaves & load balancing at each step





Keeneland (ORNL)

150M pts in 0.4s

Phil Roth @ ORNL

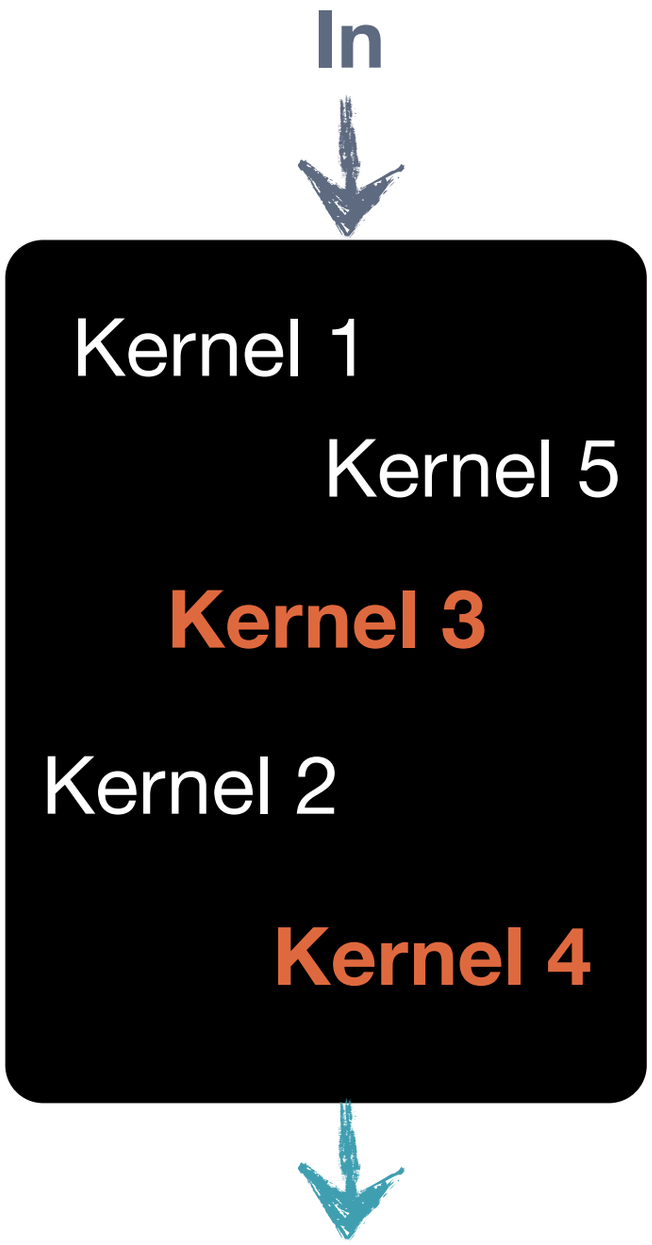
LIMITATIONS

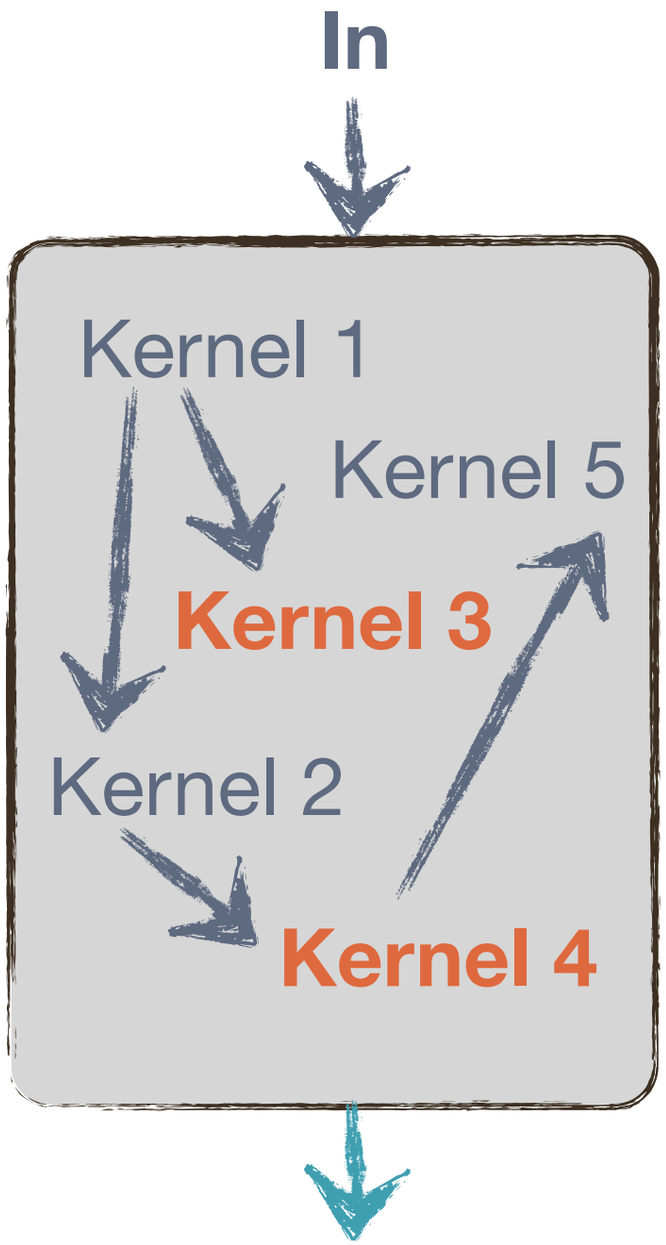
- Physics
  - Free boundaries*
  - Low volume fraction*
  - Newtonian fluid model
  - Low Reynolds numbers
- Algorithms
  - Large memory requirement for v_{local} : ~ η^3
  - No shared memory parallelization in the tree construction*
  - Need scalable data analysis*

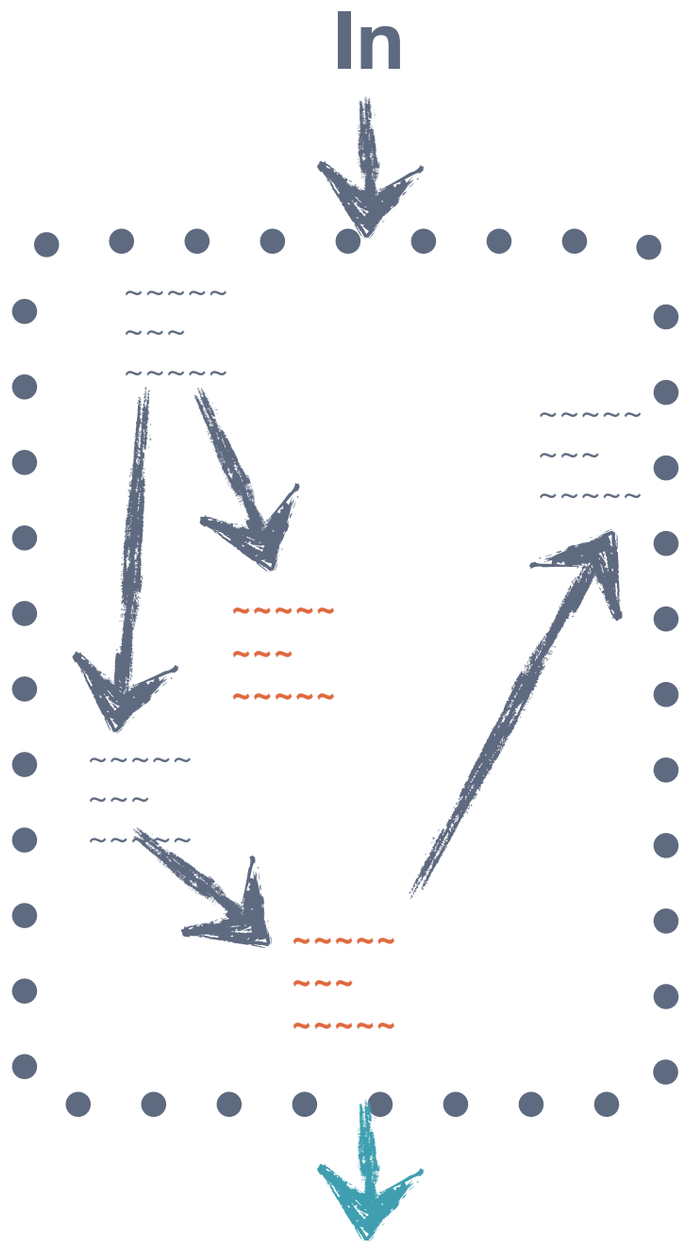
* Mathematical fix but no parallel implementation or fix in progress

- Intra-node tuning of the FMM

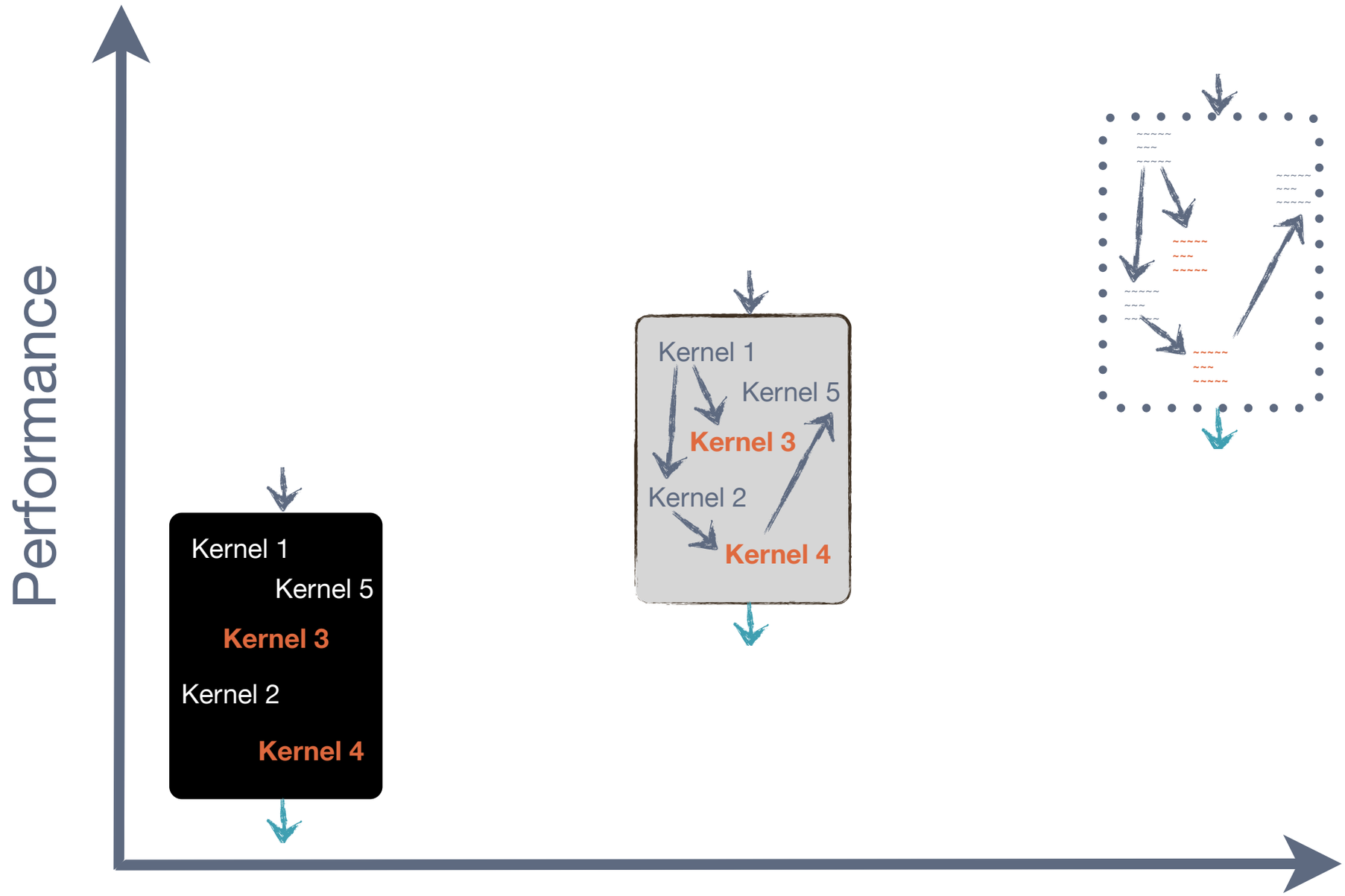
  A. Chandramowlishwaran, K. Madduri, R. Vuduc. “Diagnosis, tuning, and redesign for multicore performance: A case study of the FMM.” (SC’10)
  http://dx.doi.org/10.1109/SC.2010.19





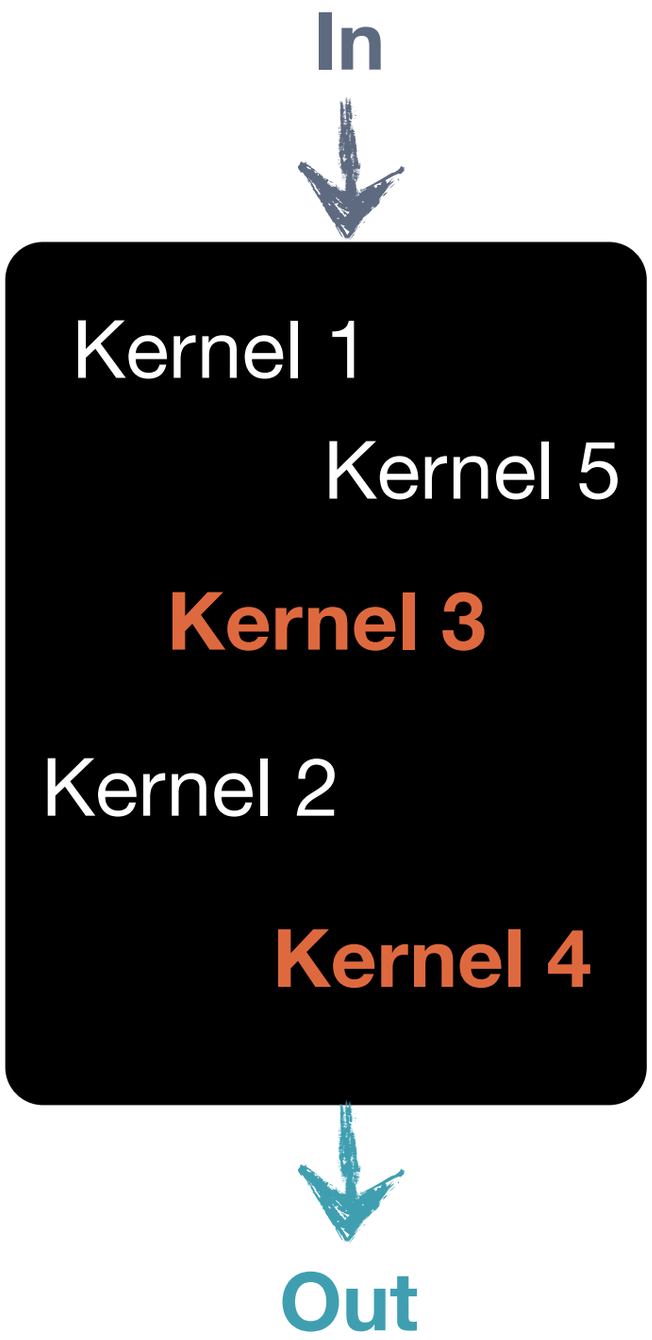


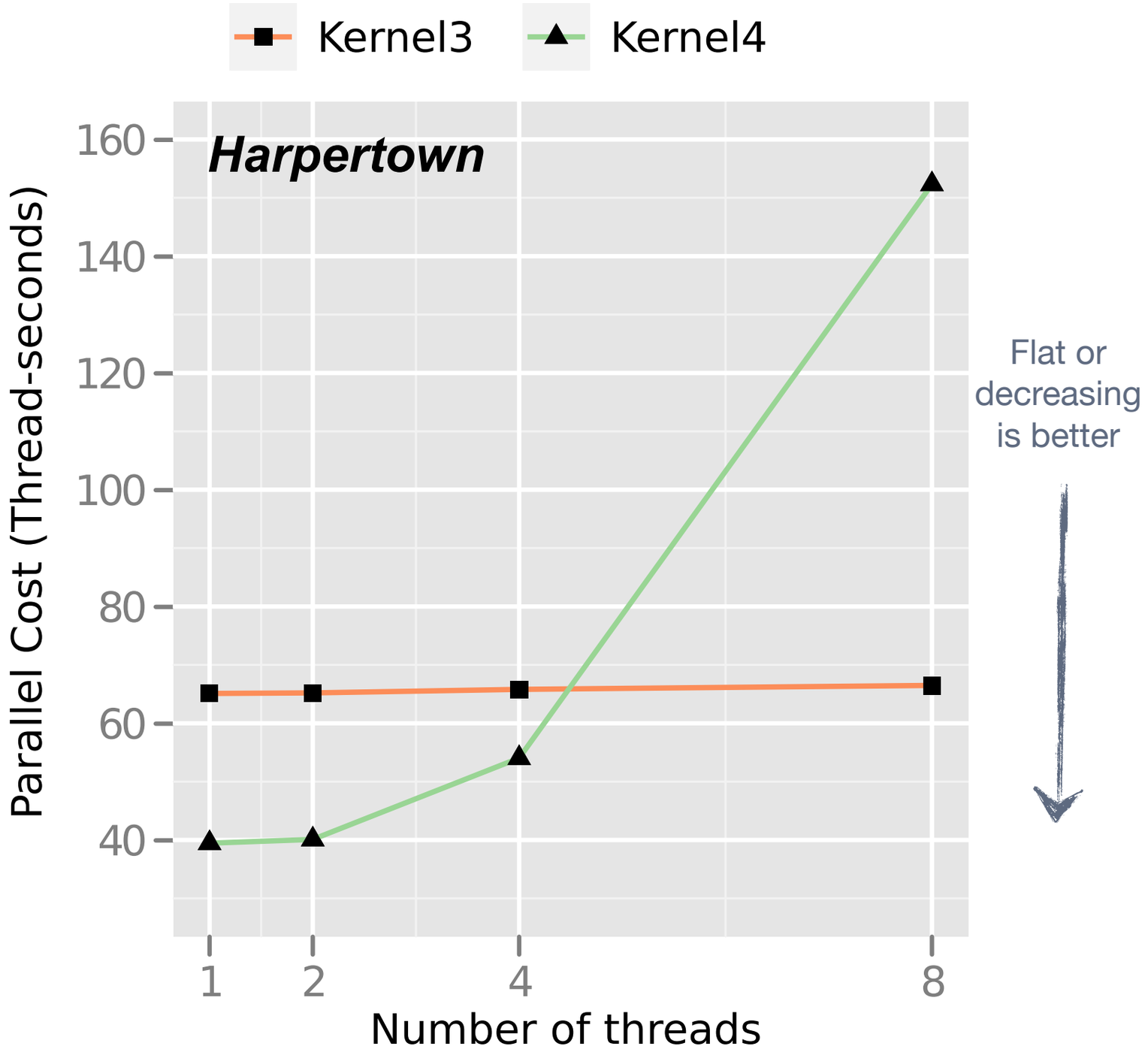
How to find and fix bottlenecks?



A NOTIONAL TUNING PROCESS

Achieved performance increases as we increase our knowledge of the details of the application, from “black box” to “full knowledge.”

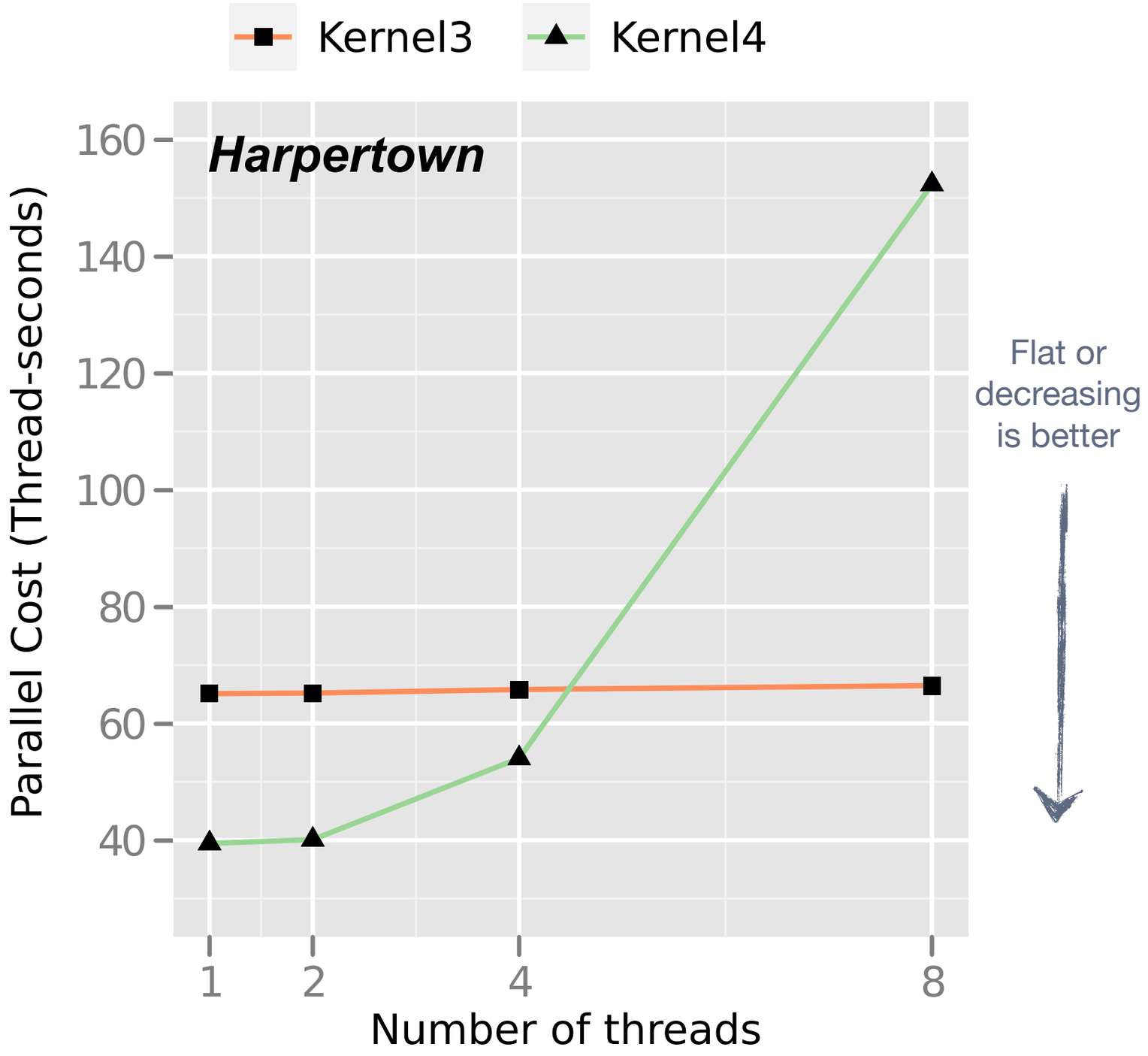




STAGE 1: BLACK BOX

Assume simple profiling and no code changes.

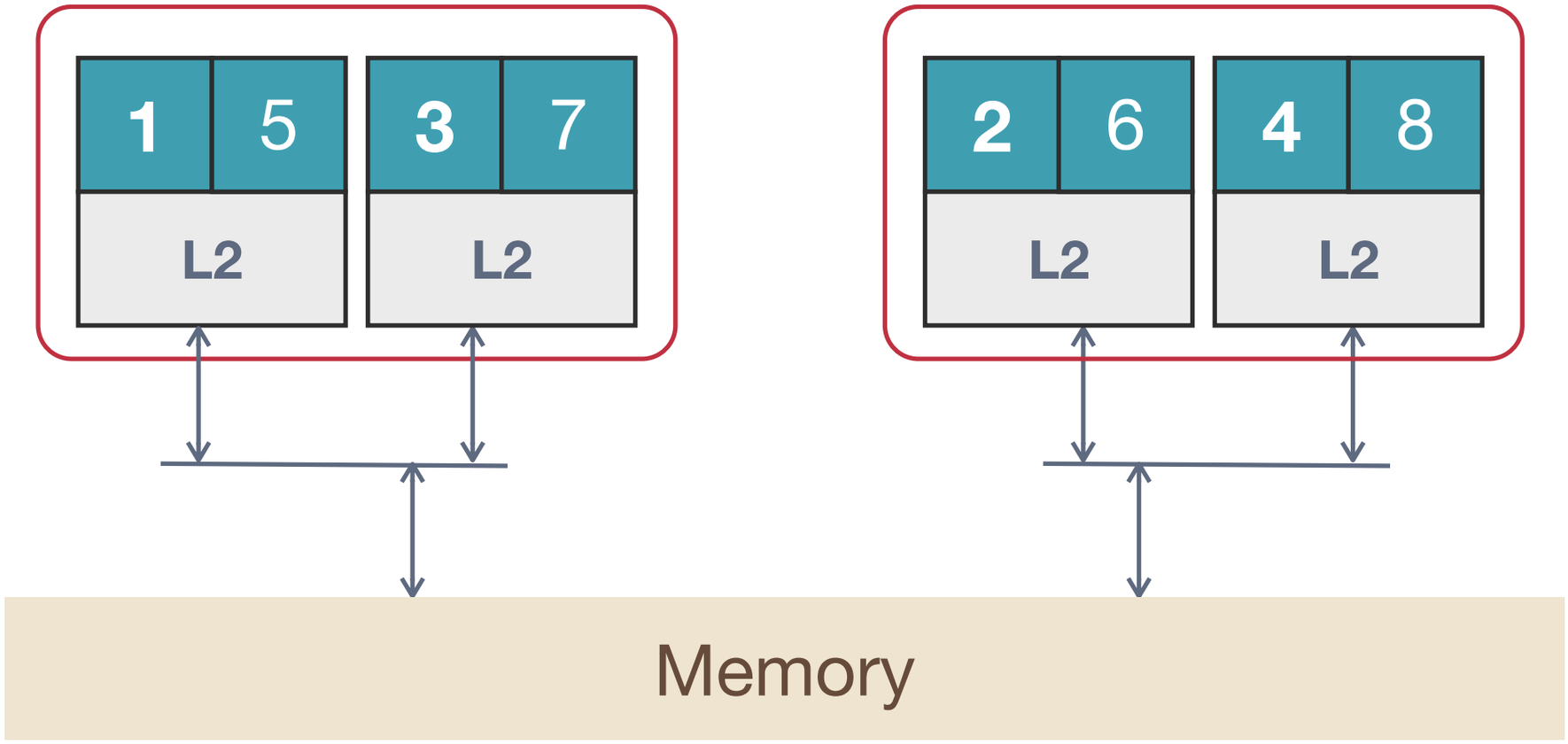
- Observe: K4 scales poorly
- Measure intensity
  - K3 = compute-bound
  - K4 = memory-bound
- Hypotheses:
  - Load imbalance?
  - Memory contention? Cache or bandwidth?



STAGE 1: BLACK BOX

Assume simple profiling and no code changes.

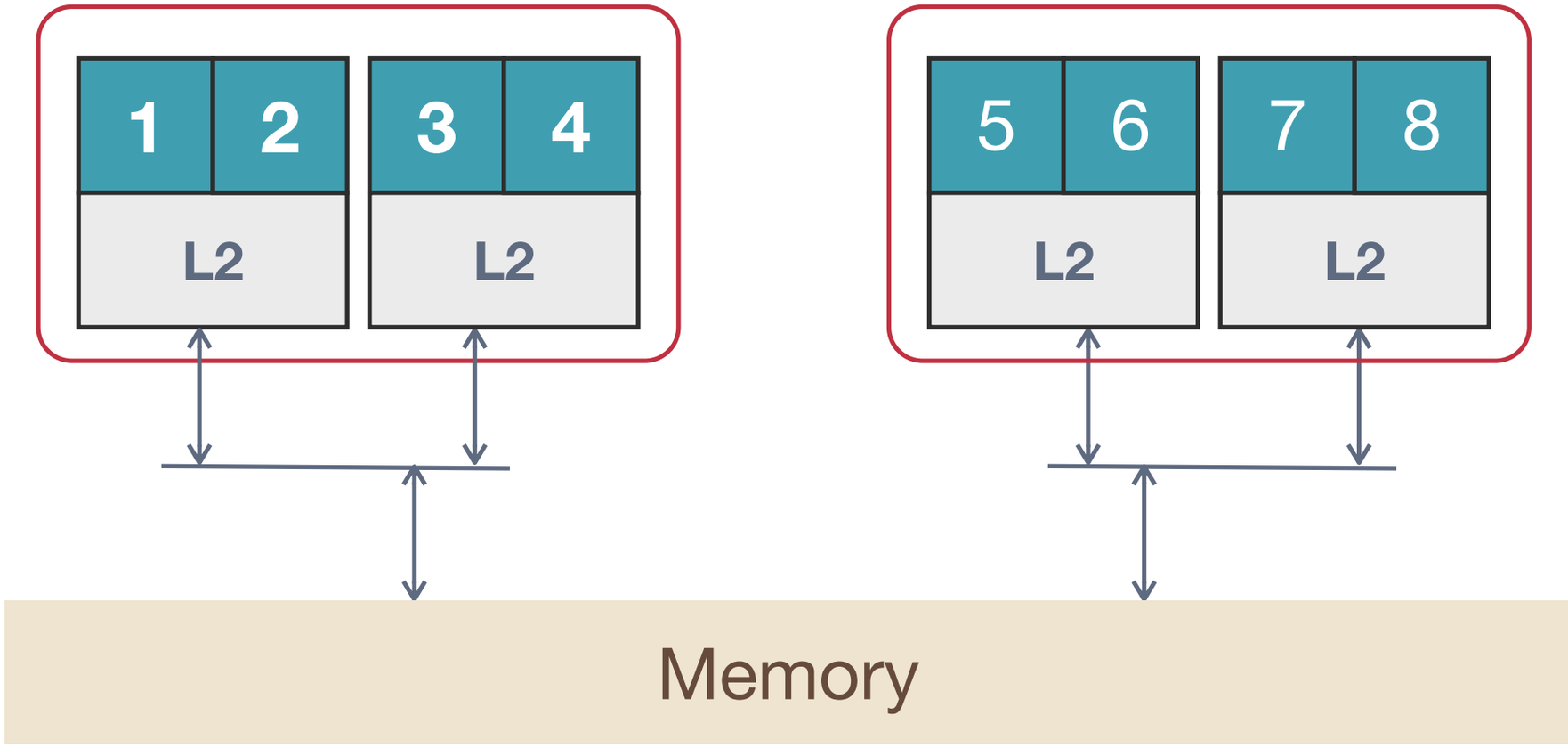
Intel Harpertown



threads = 8

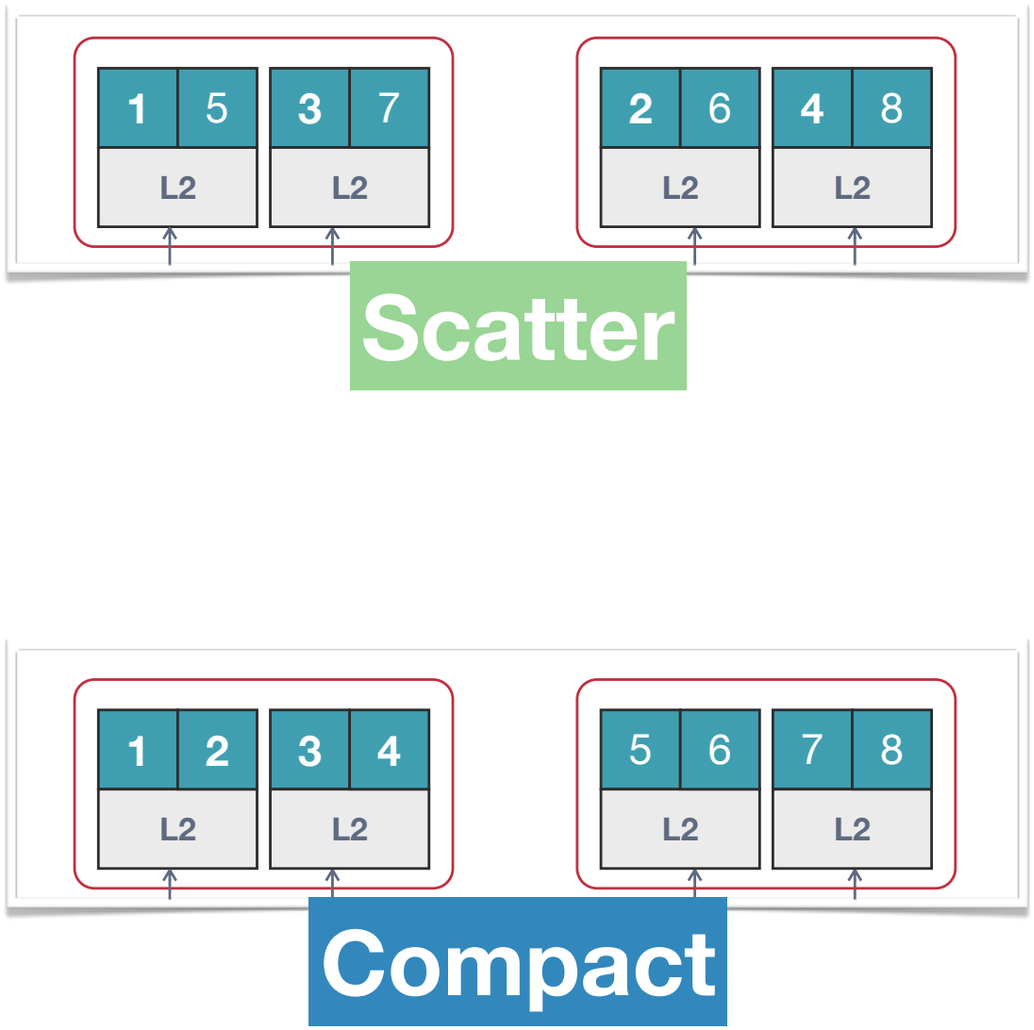
OpenMP *scatter*

Intel Harpertown



threads = 8

OpenMP *compact*

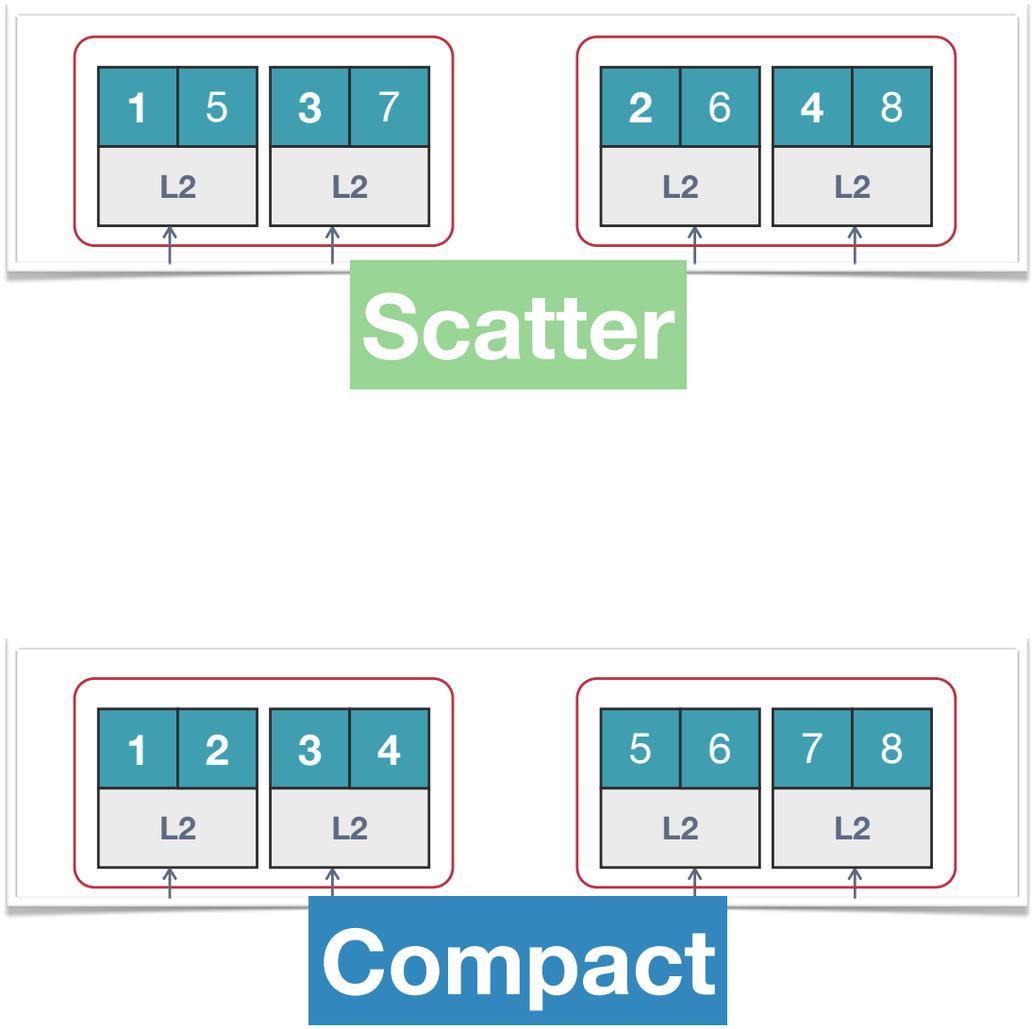


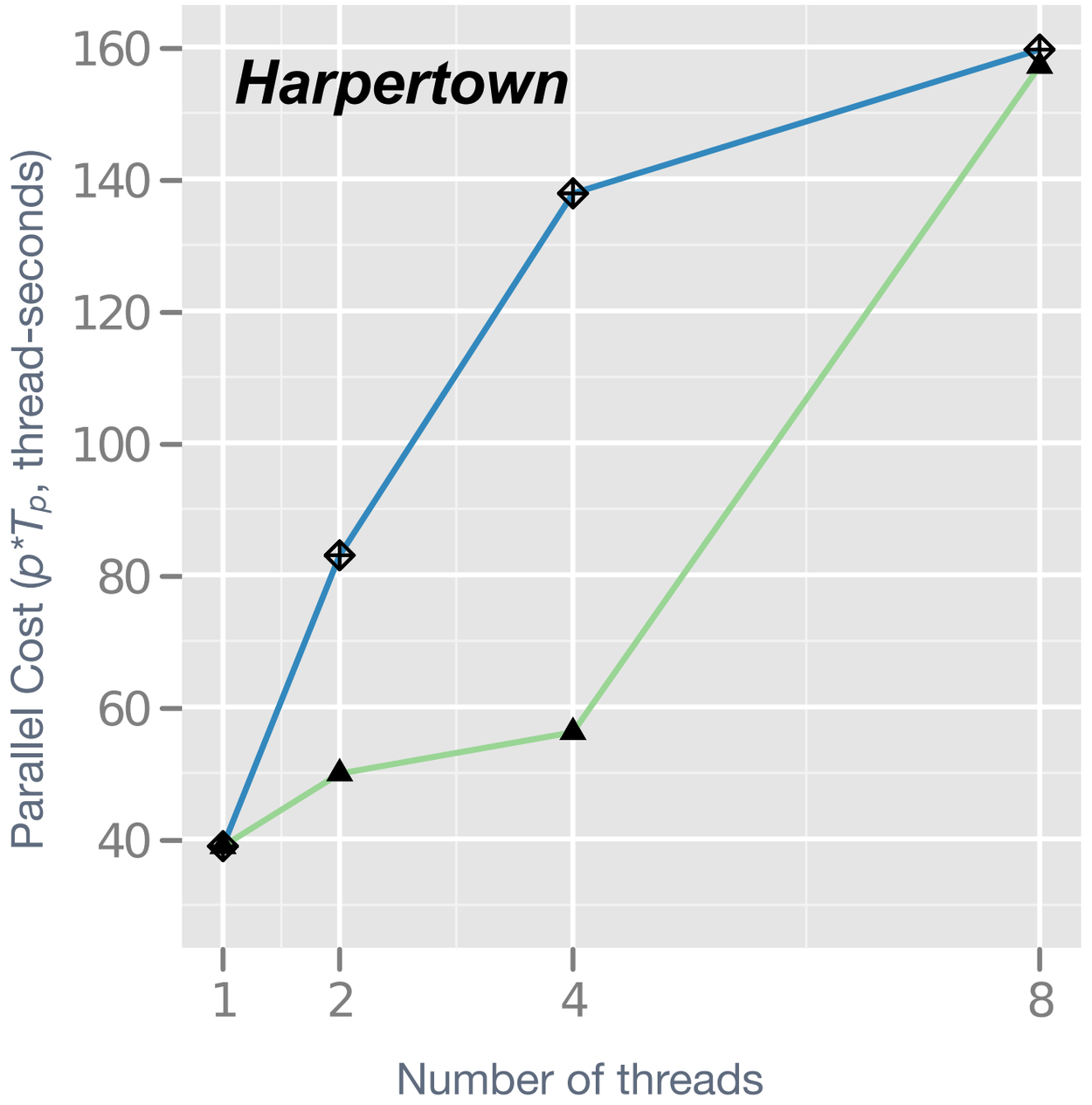
Parallel Cost ($p*T_p$, thread-seconds)

Number of threads

VARYING THREAD BINDING STRATEGY

Assume simple profiling and no code changes.





Varying Thread Binding Strategy

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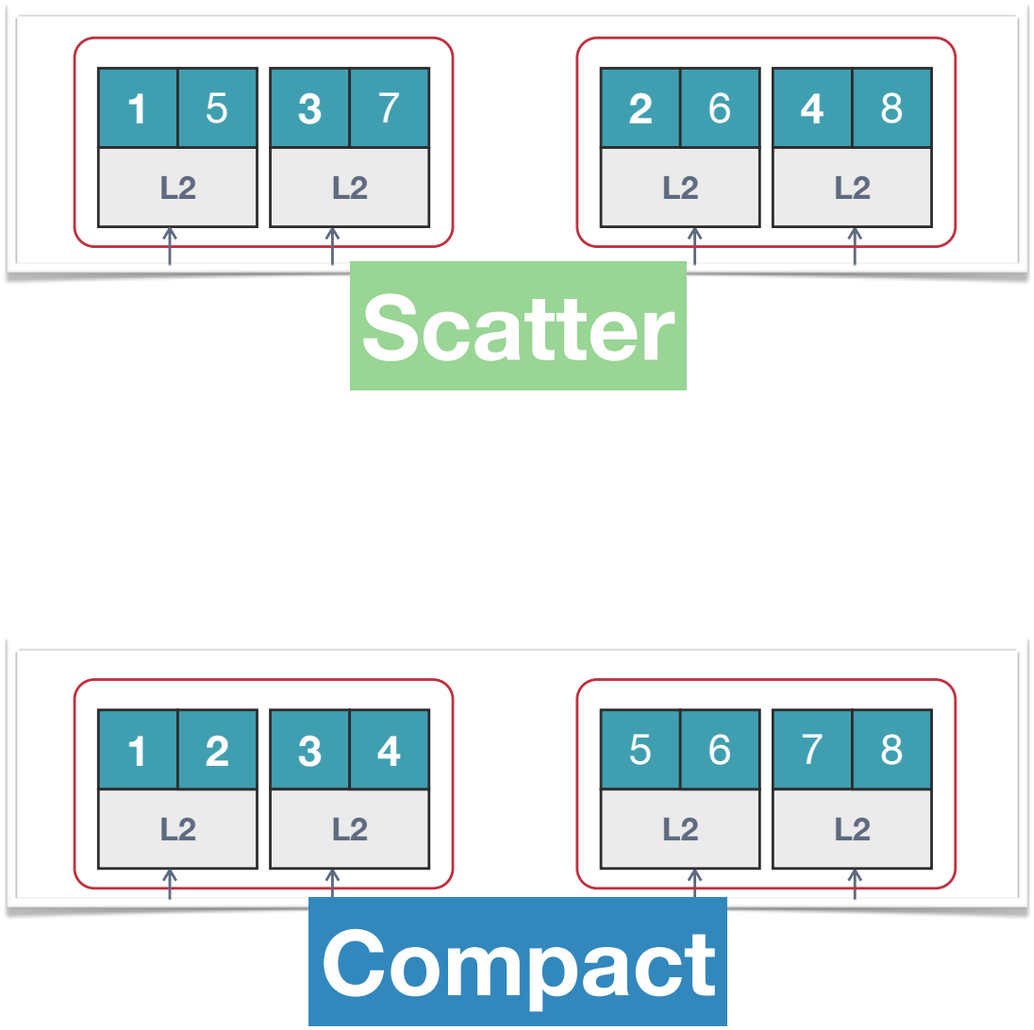

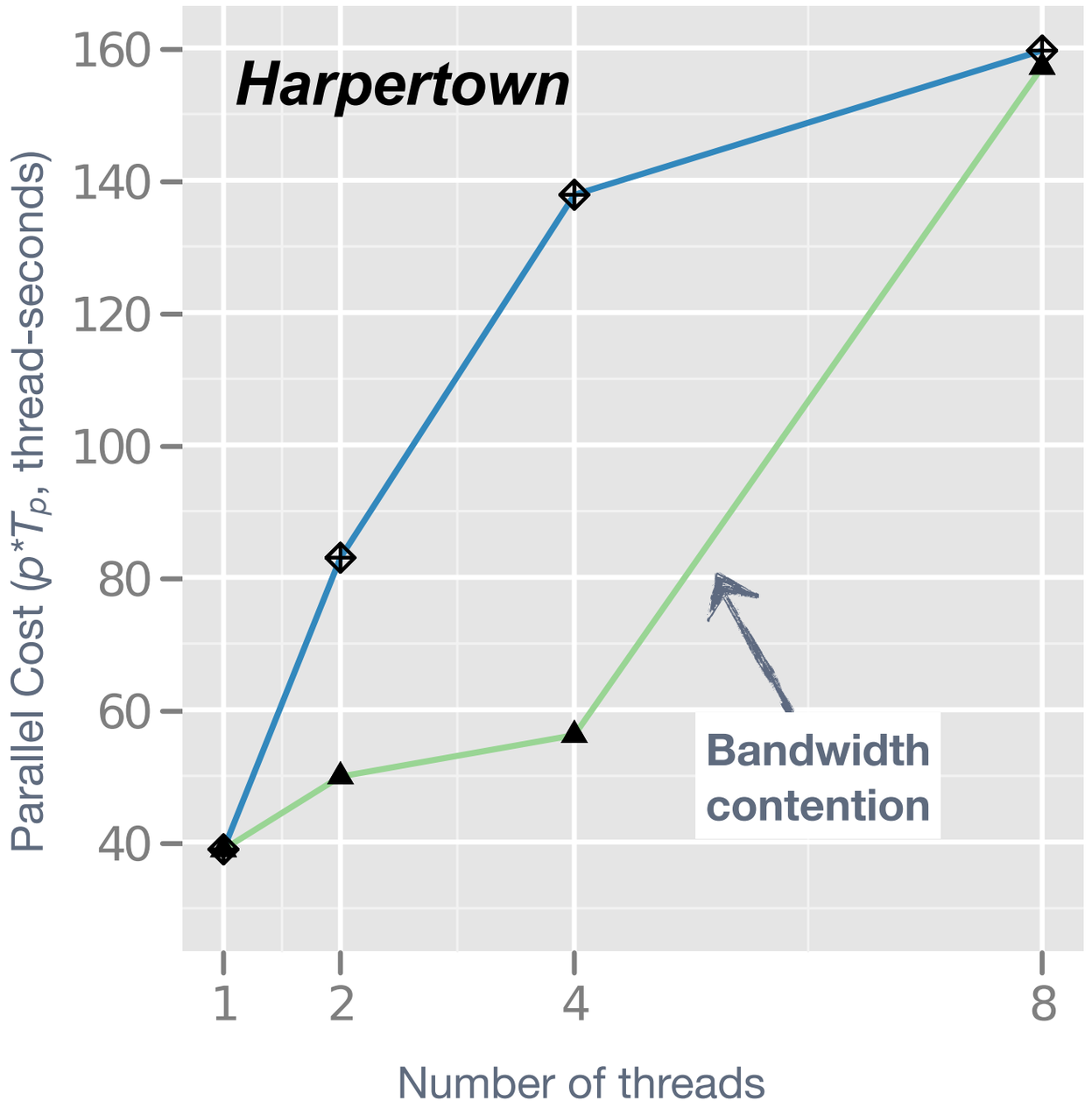

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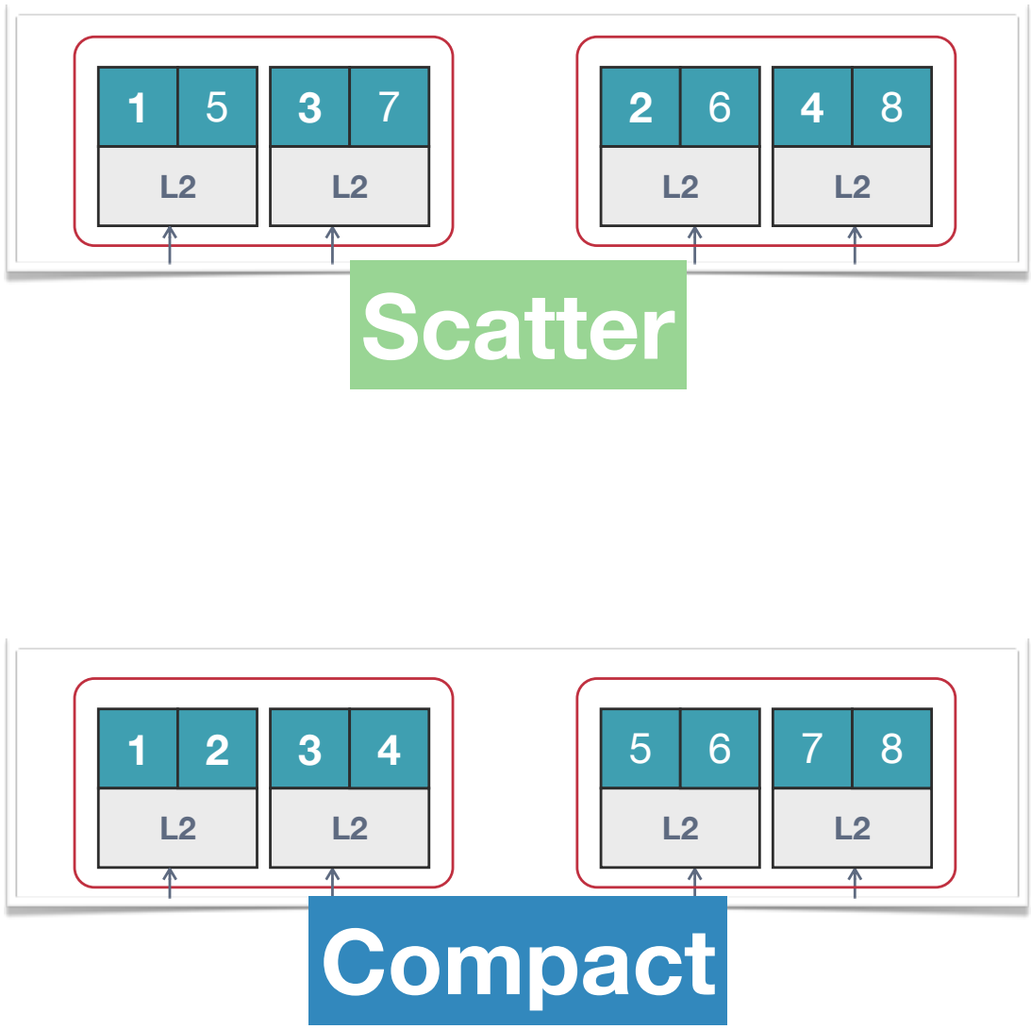
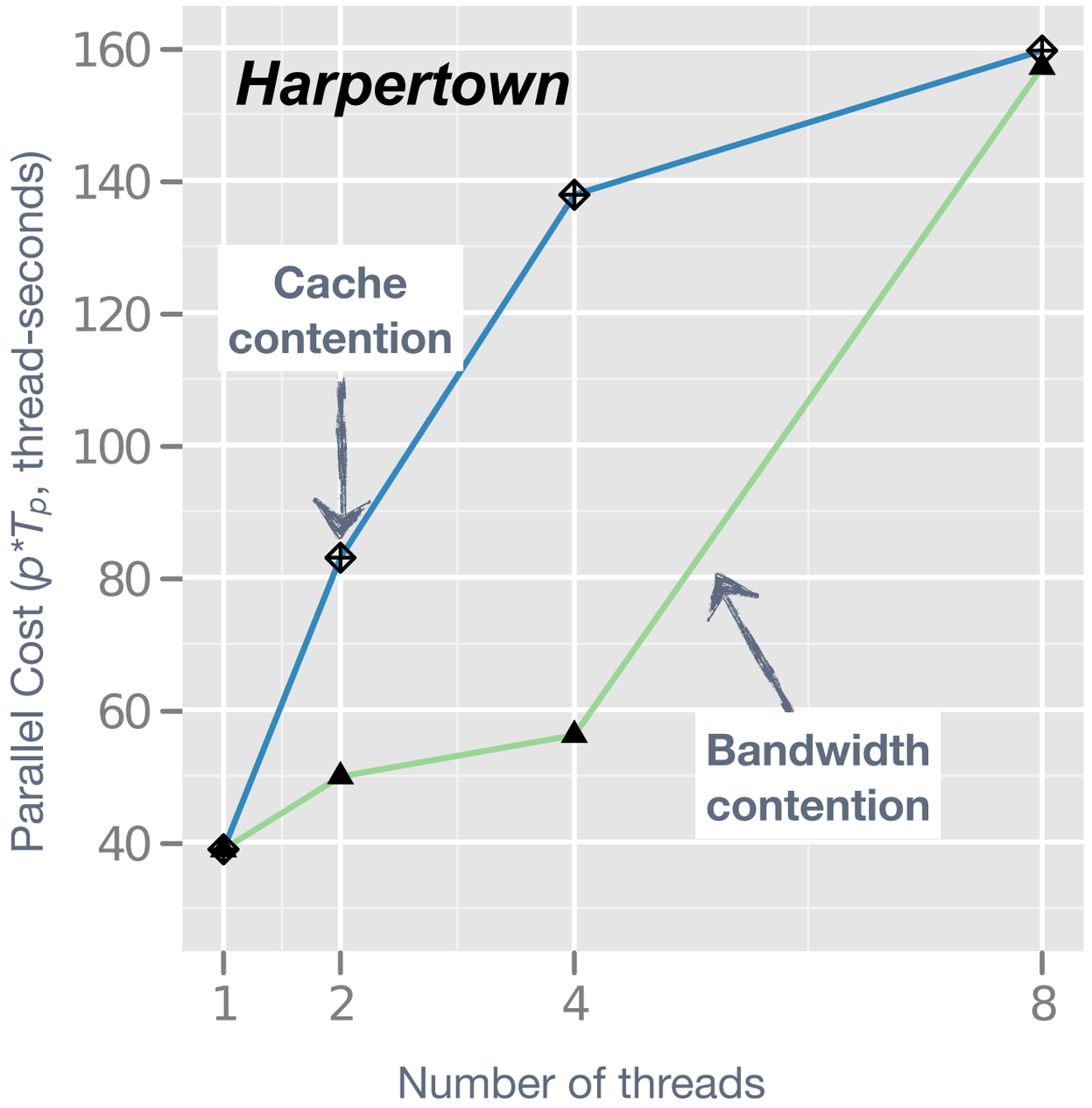
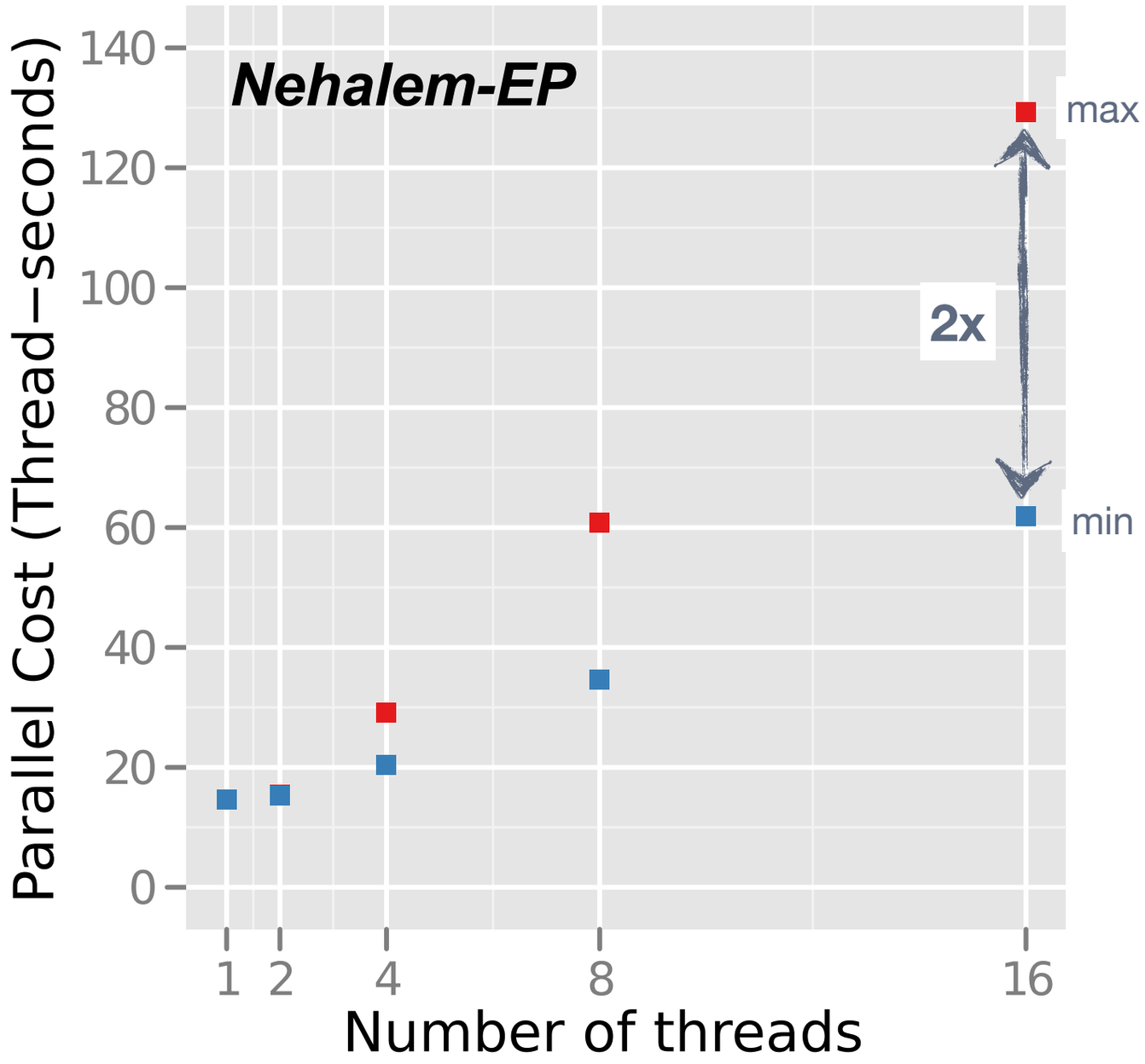




Varying Thread Binding Strategy

Assume simple profiling and no code changes.

- On a 4 x 4-core NUMA system, observe load imbalance in K4 where previously there had not been one
- Observe identical flop instruction counts, suggesting memory cost imbalance
- Possible quick fixes
  - *Guided* scheduling
  - NUMA-aware allocation



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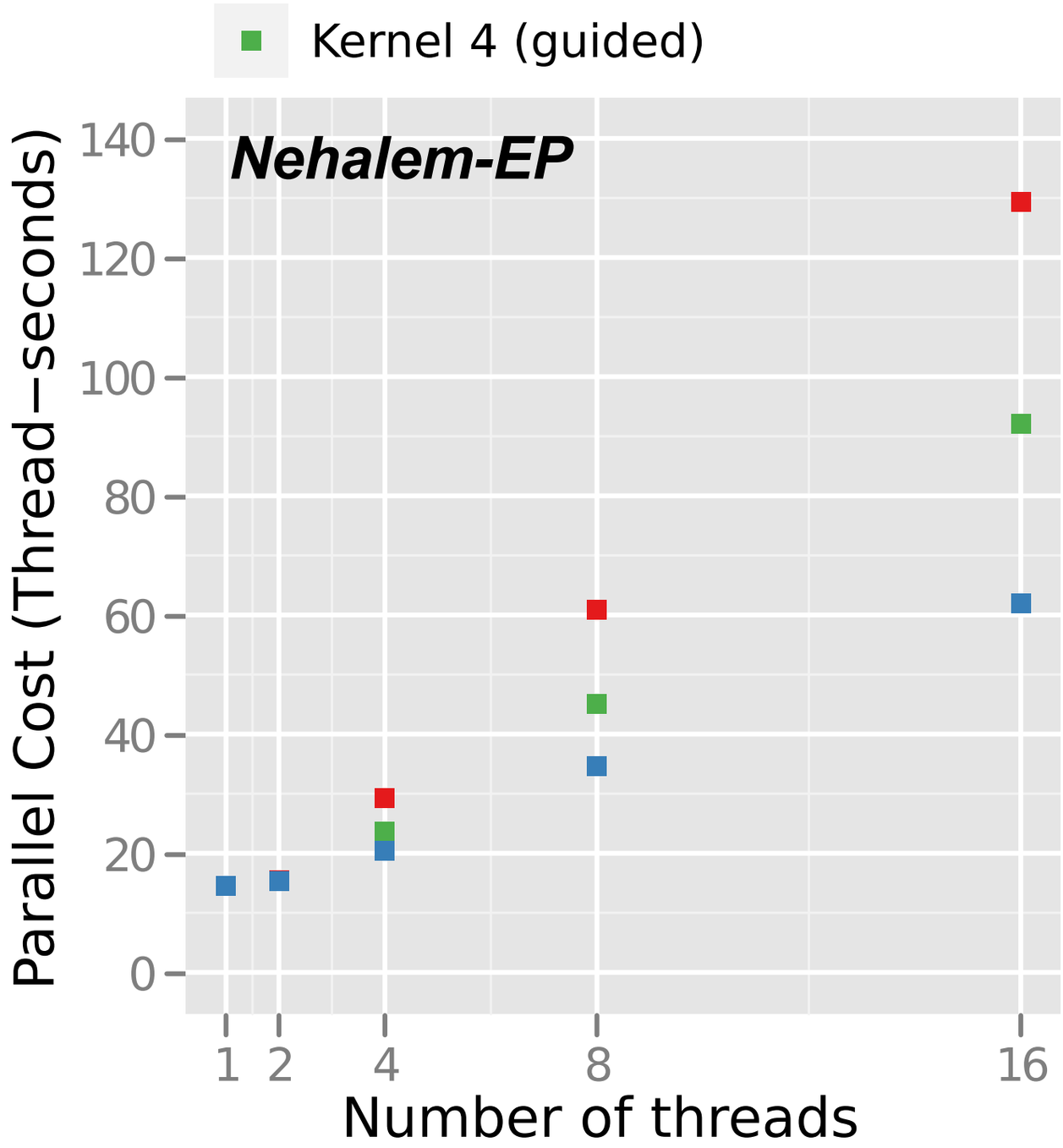

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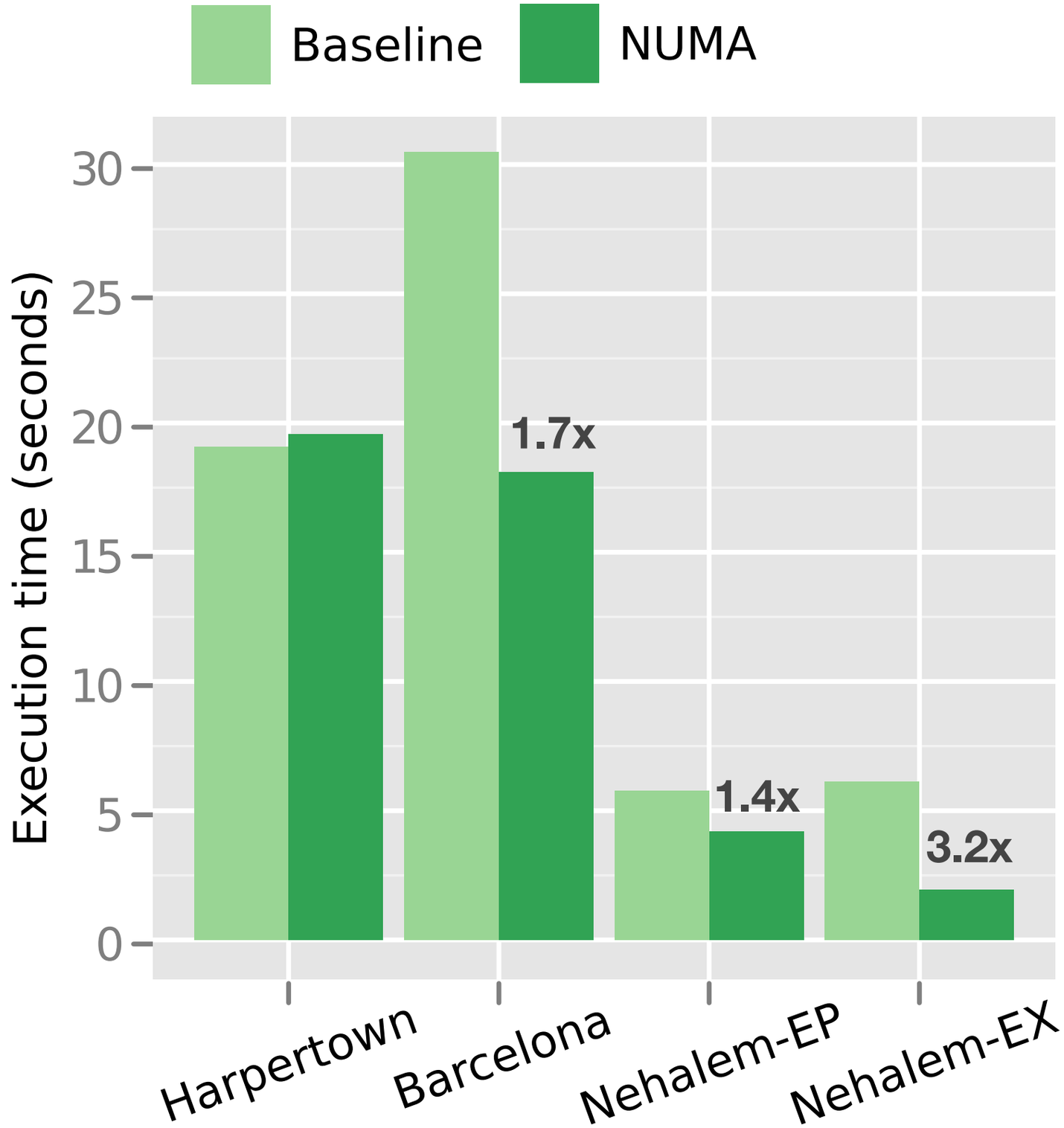

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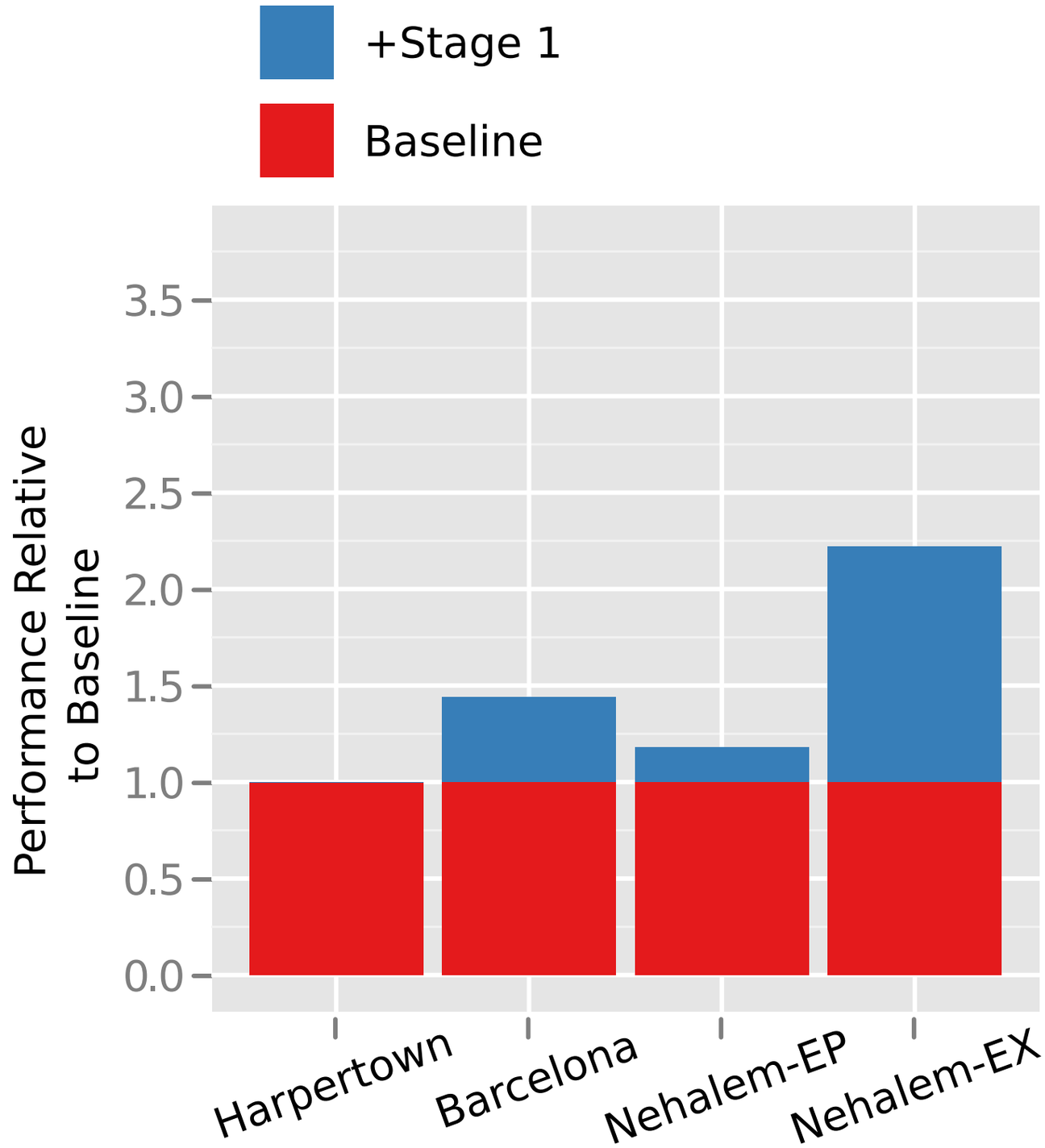

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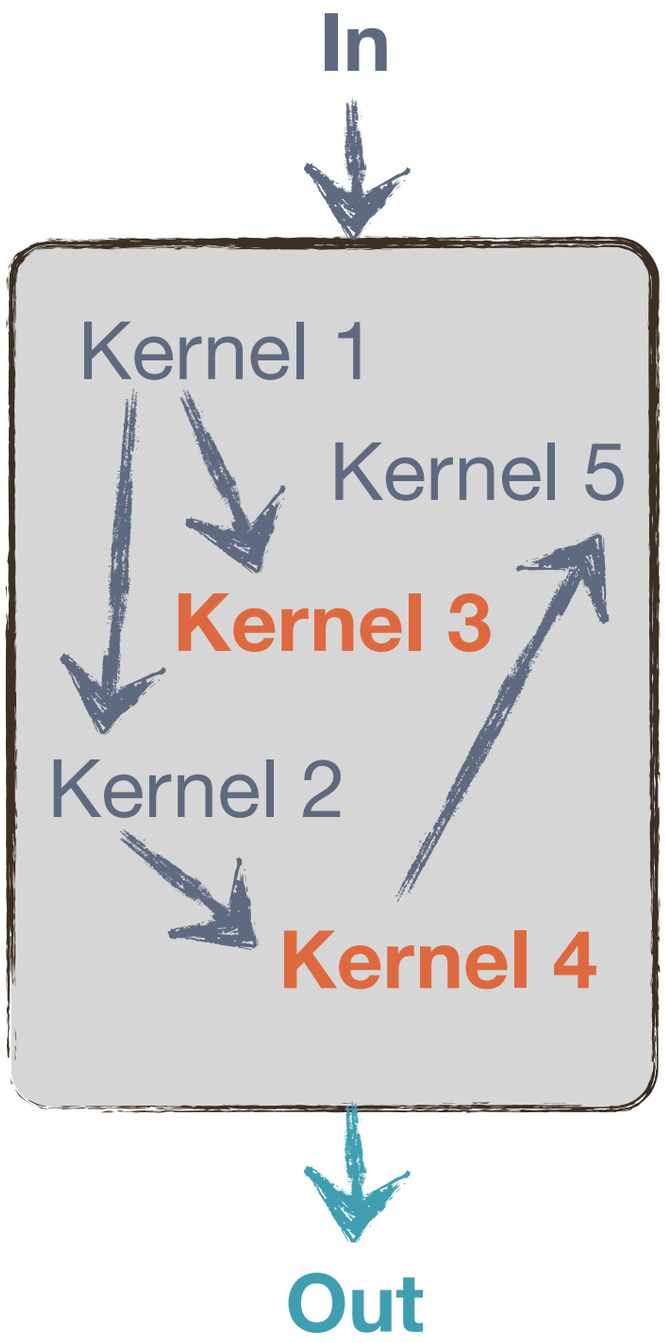
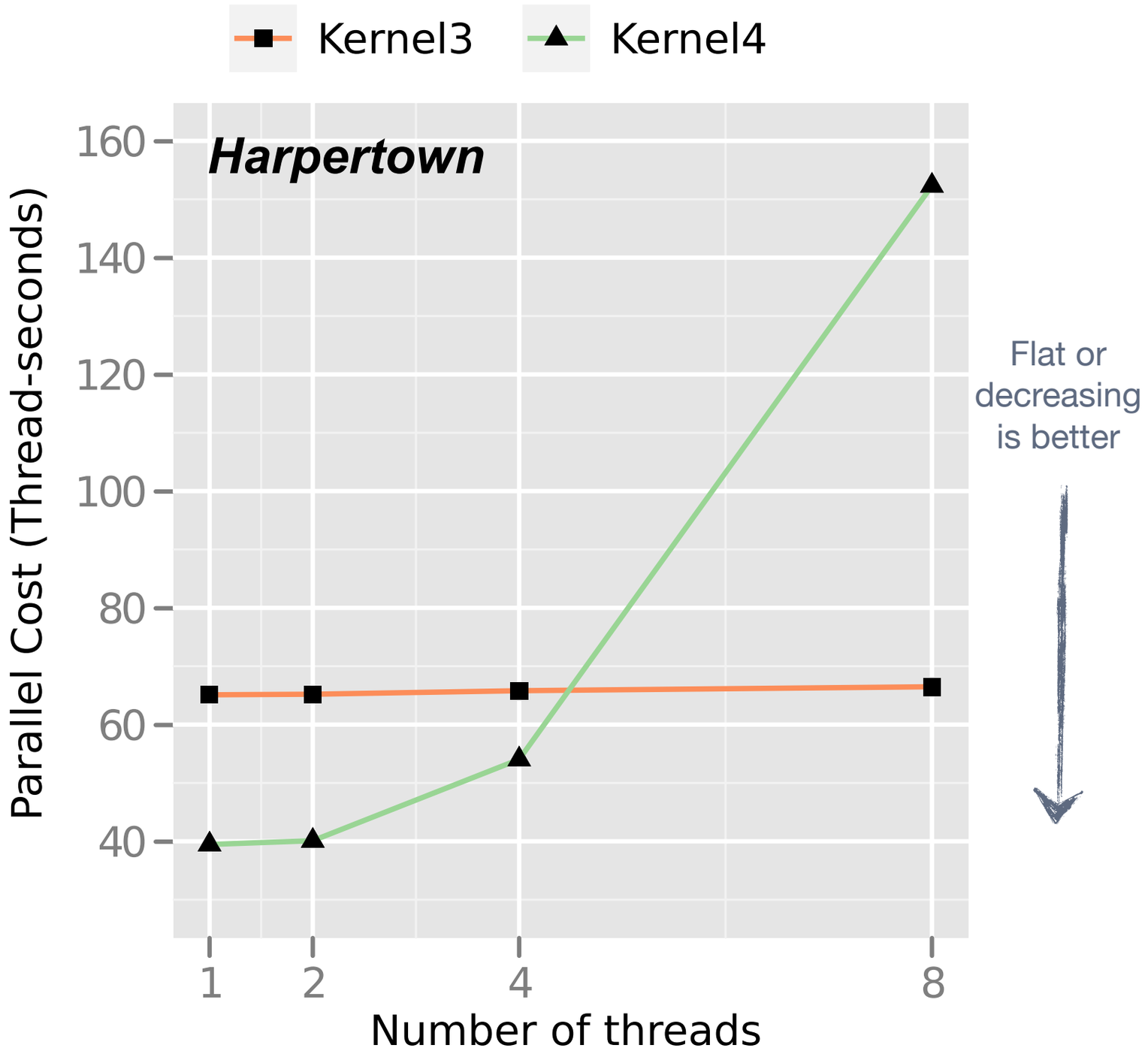
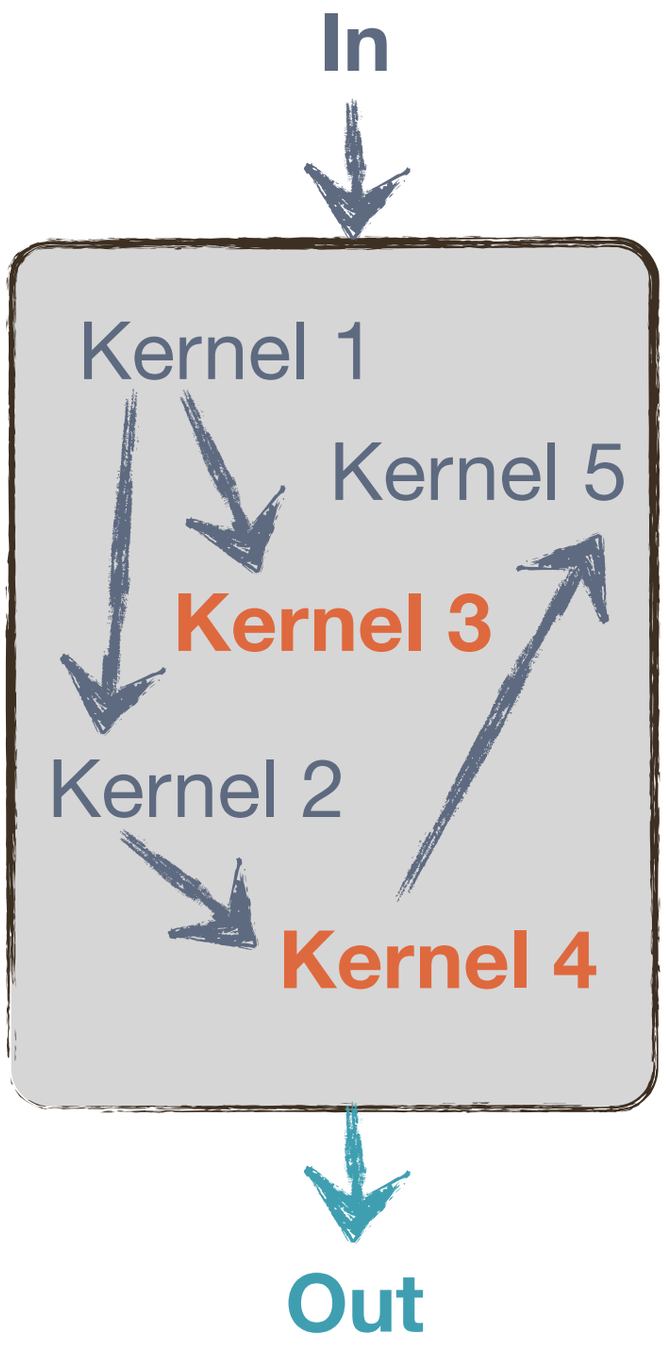
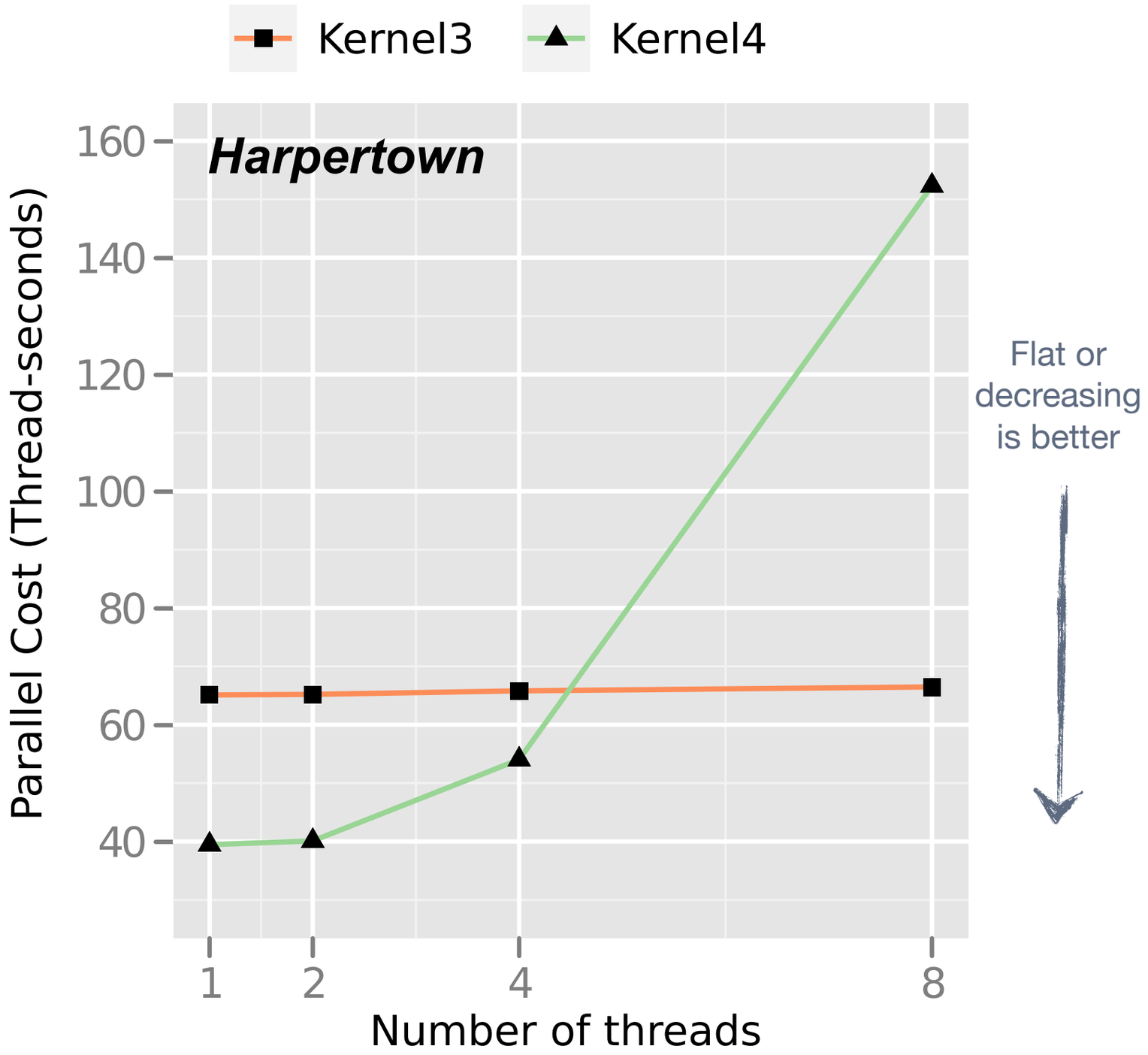




STAGE 2: DEPENDENCE

Assume additional knowledge of the task dependency structure





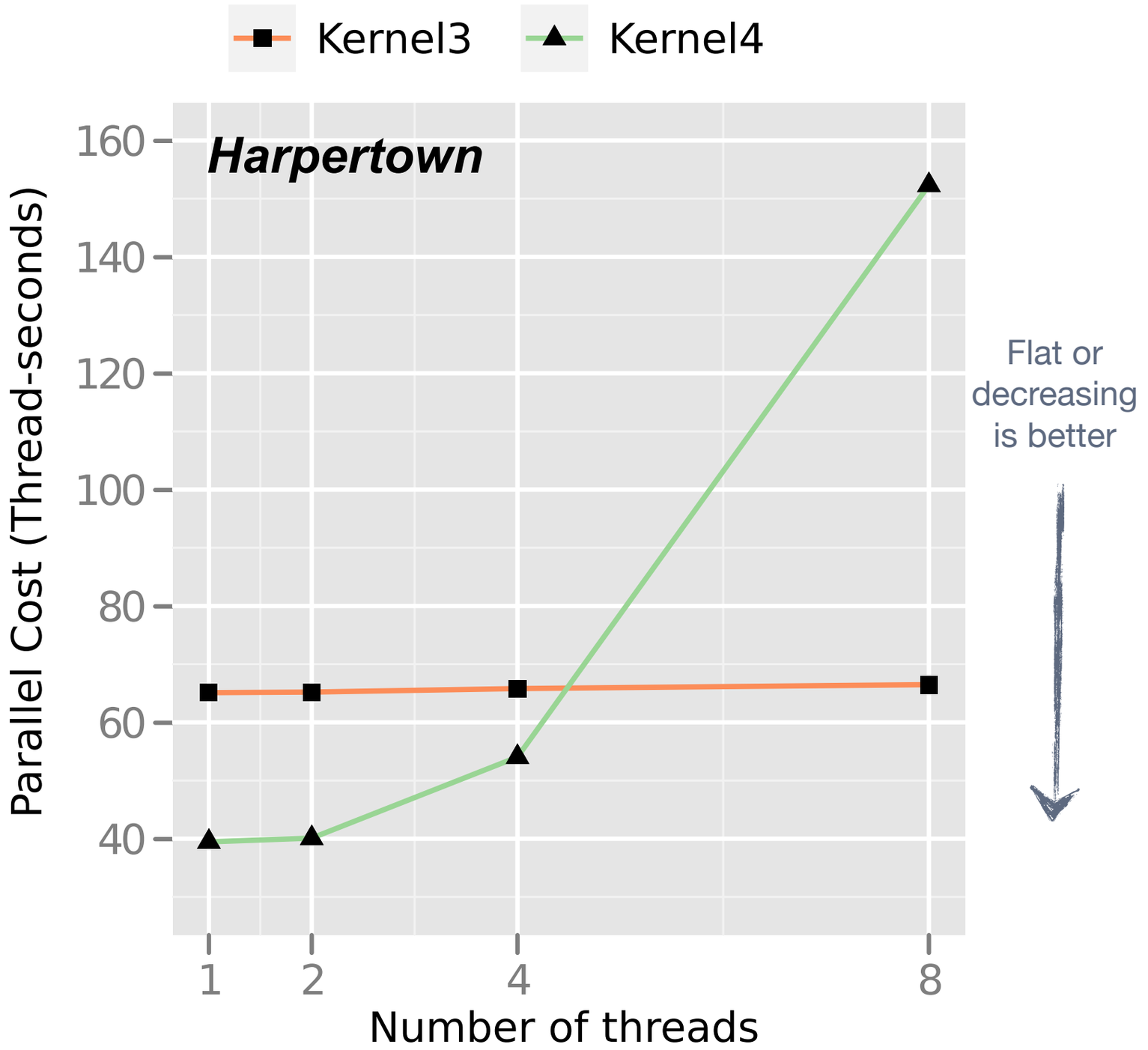
STAGE 2: DEPENDENCE

K3 and K4 are independent. Running them **concurrently → up to 2x** improvement.

- **Idea 1**: Try simultaneous multithreading (**SMT**) execution

- *Intuition*: K3 is compute bound while K4 is memory bound, so there will be no contention for the same processor functional units

- Only works on Nehalem class systems, which implement SMT



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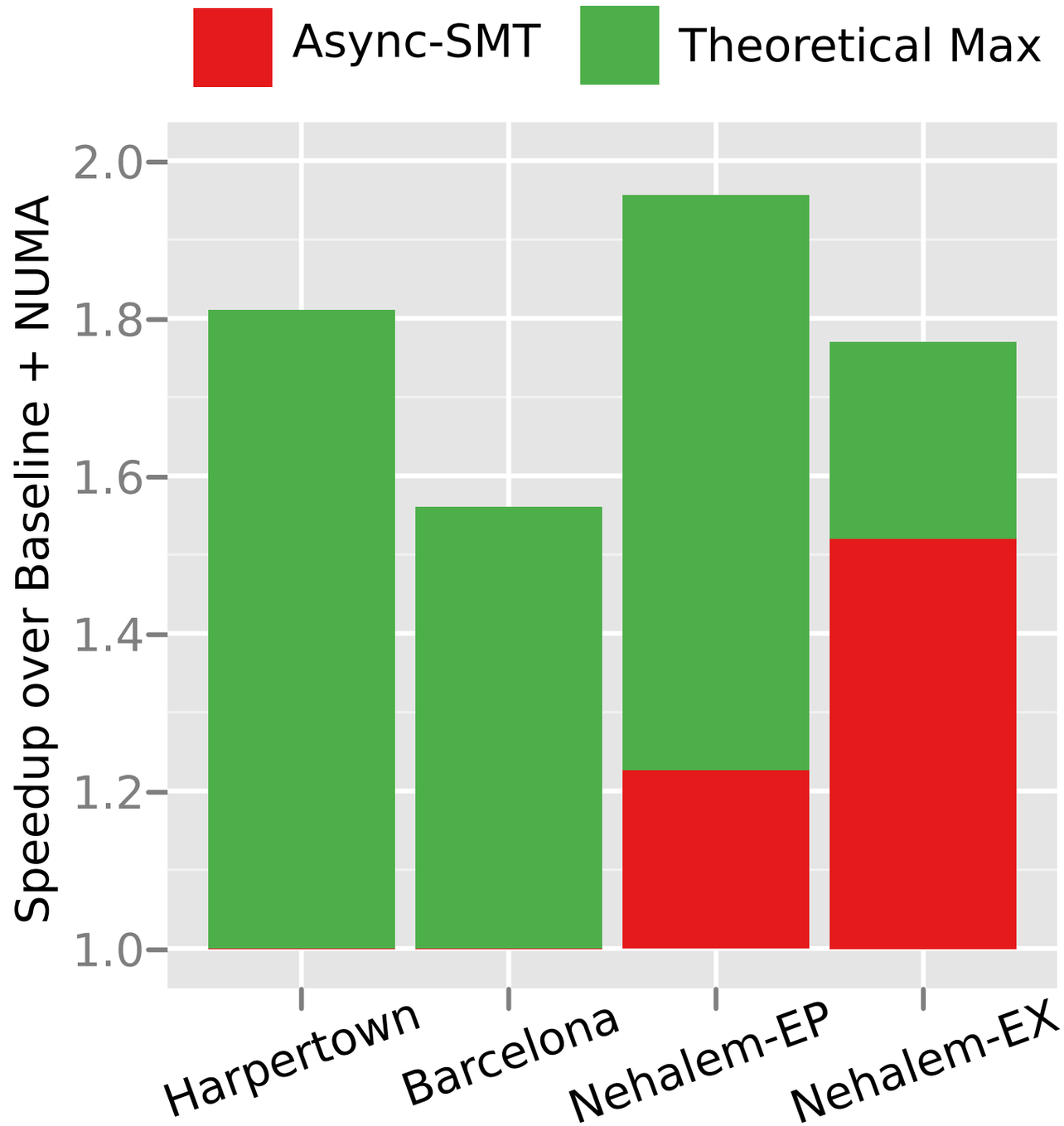

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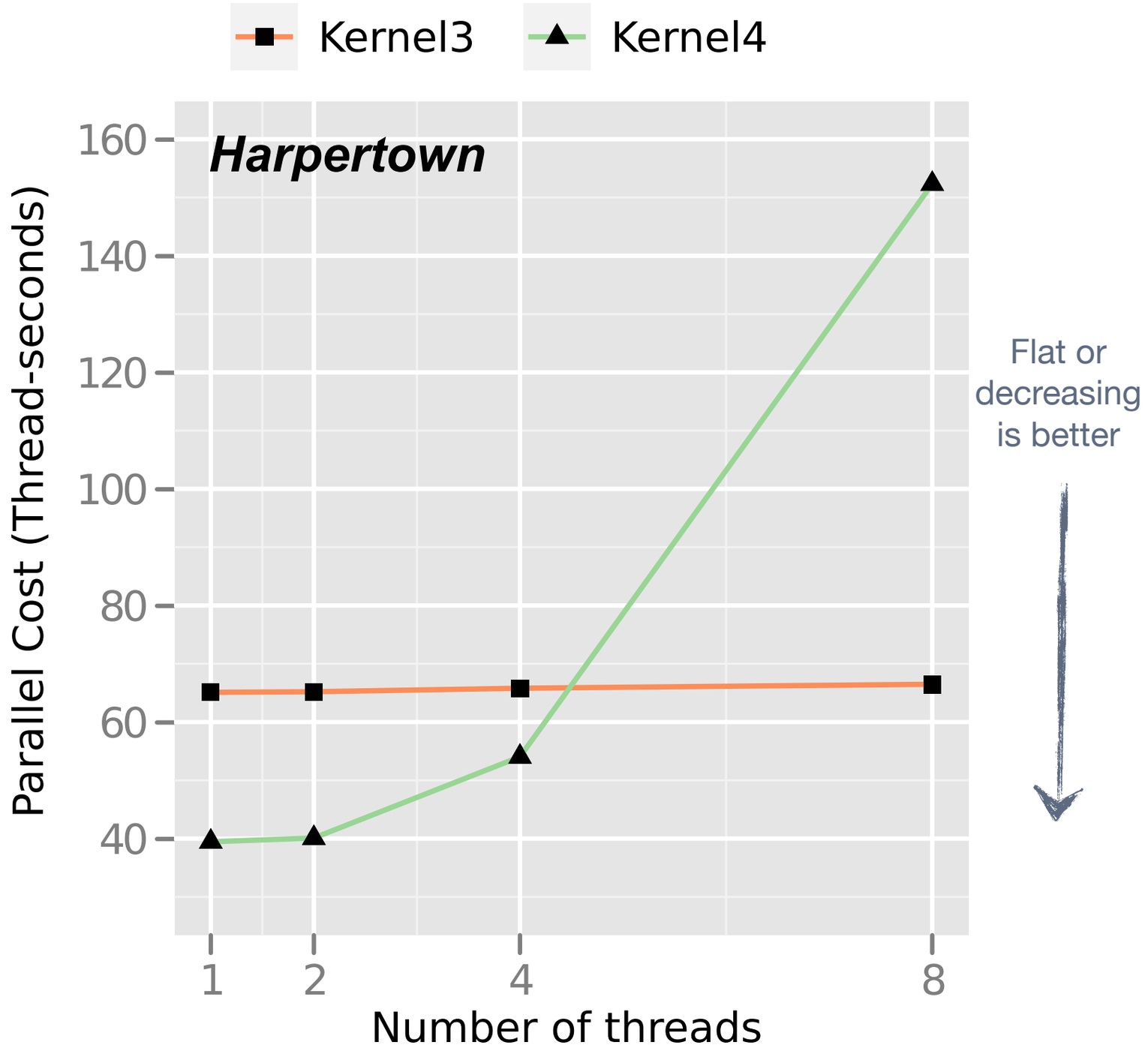
- That is, run K4 up to its scalability limit, and use remaining cores for K3



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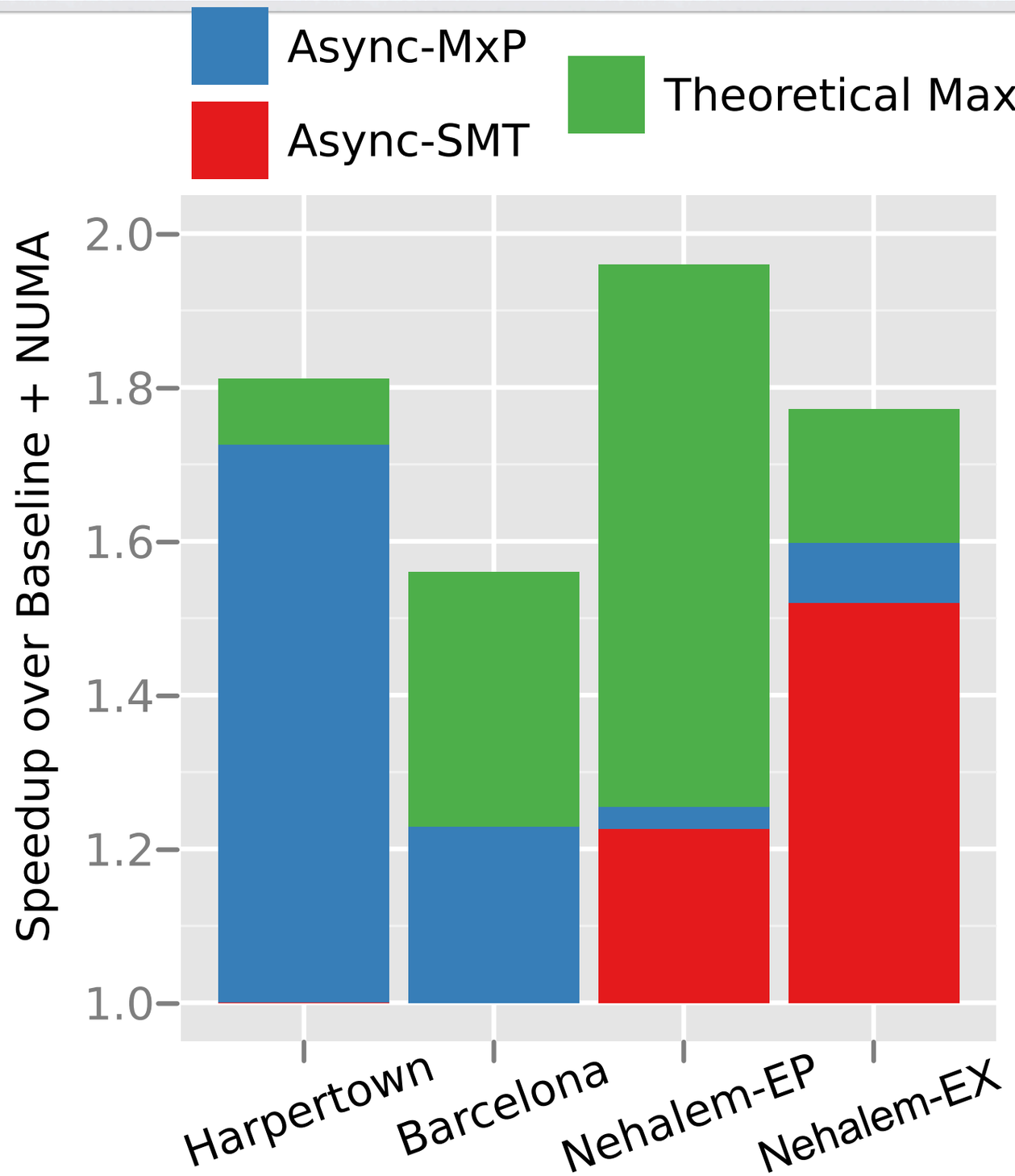
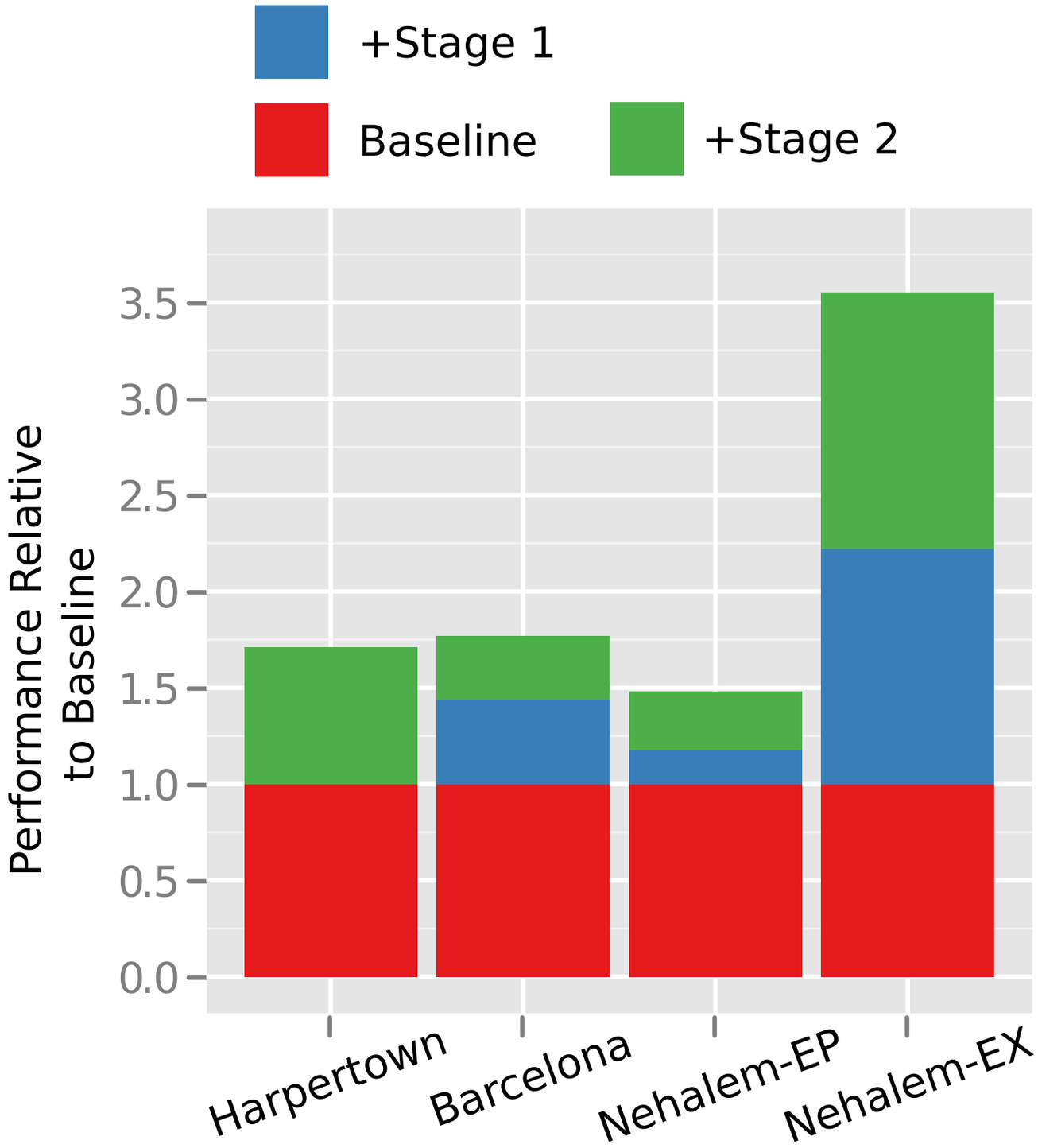


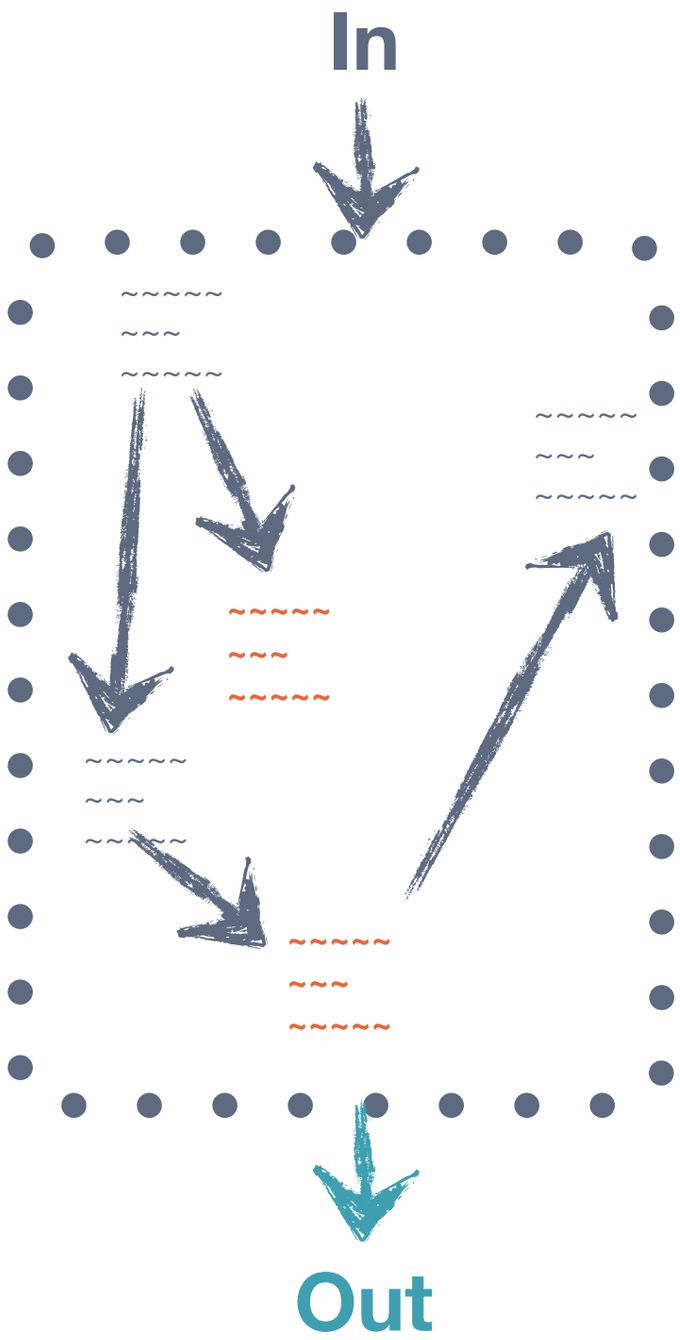
STAGE 2: DEPENDENCE

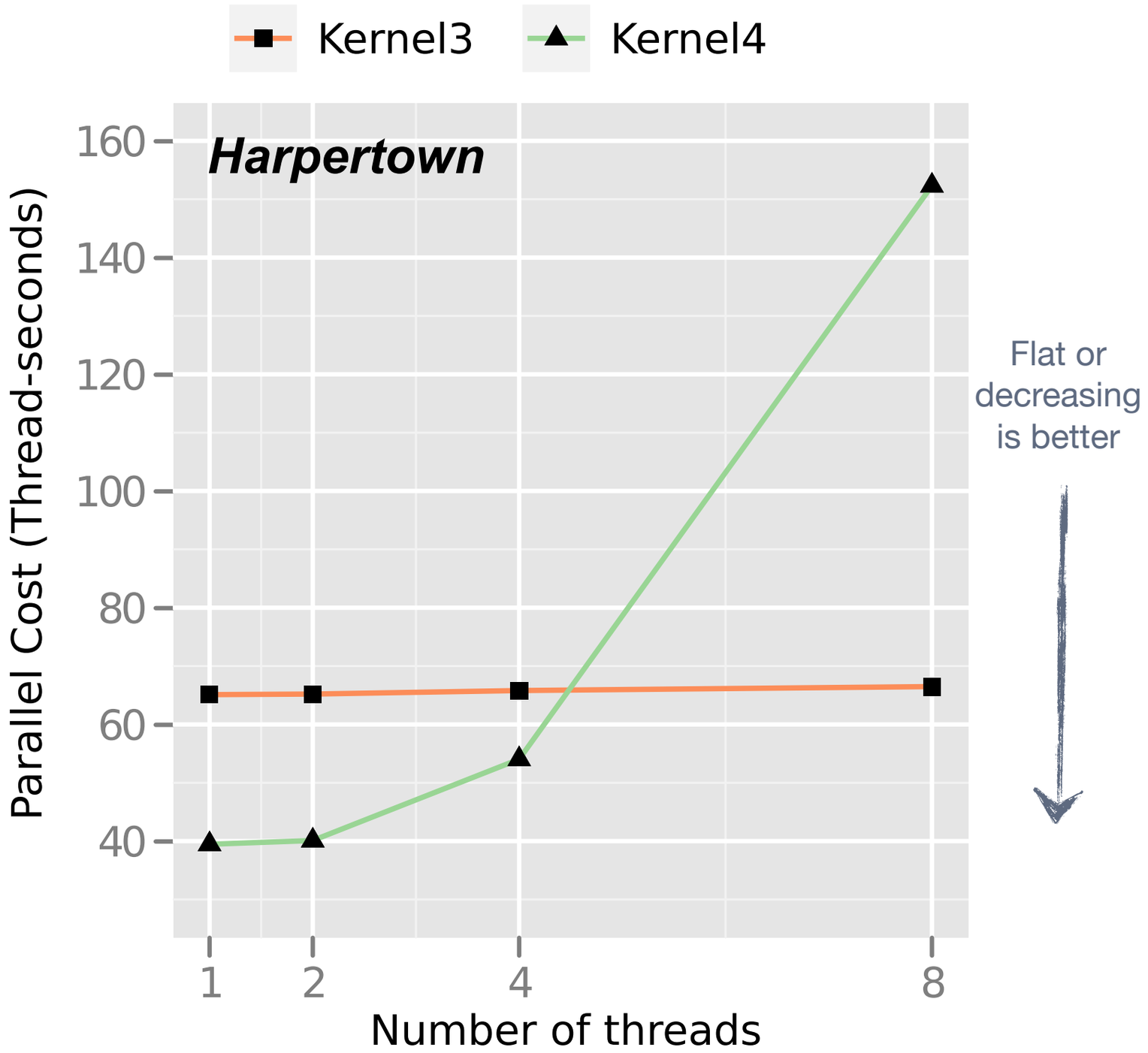
1.2—1.7x improvements possible, regardless of SMT availability



STAGE 2: DEPENDENCE

More extensive code changes but still no “deep” knowledge of code required.





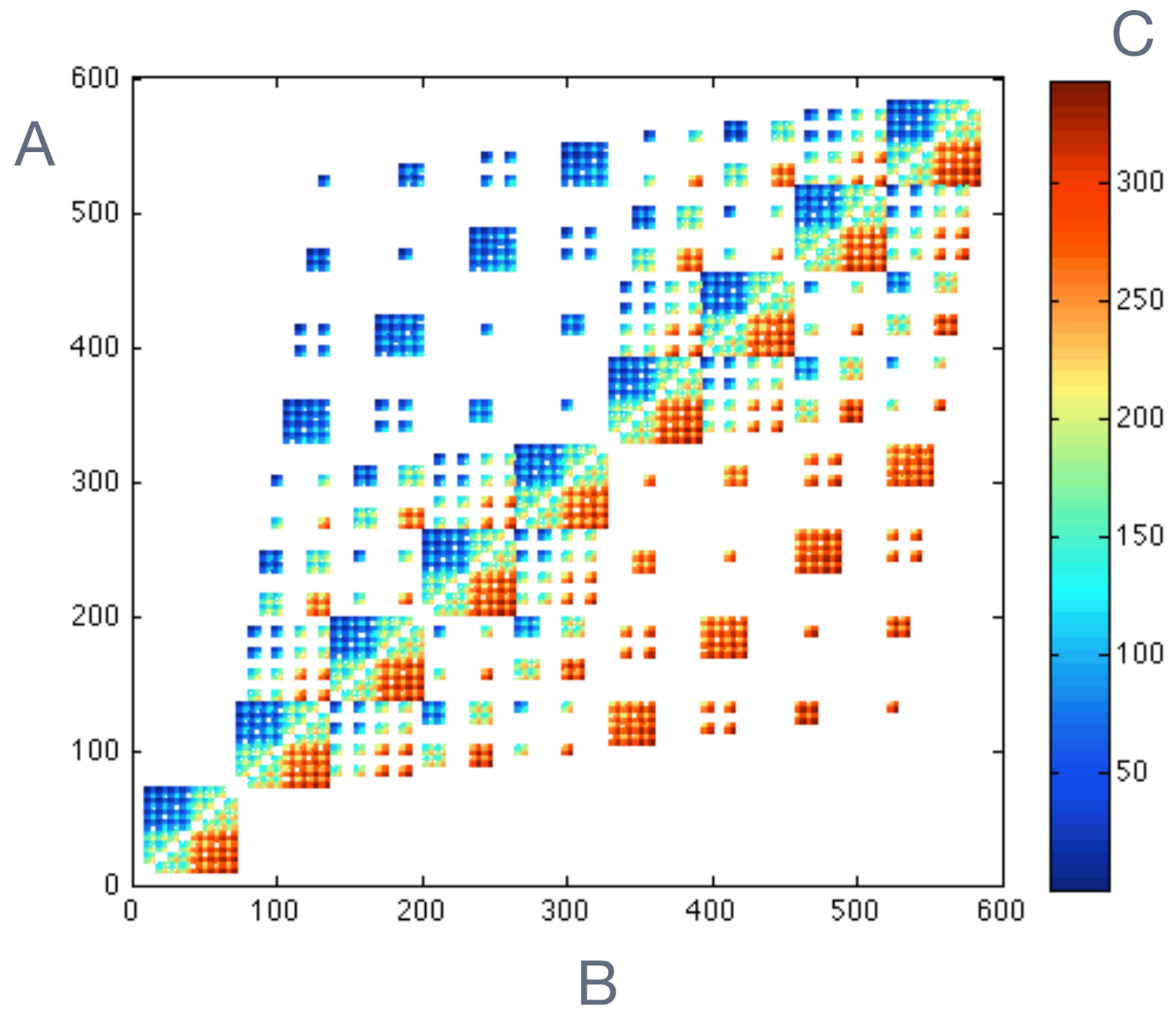
STAGE 3: ORACLE

Assume full knowledge of data access patterns, algorithms, and code

- **Example:** Full knowledge of data access pattern of K4

- Three data arrays, A, B, and C
- Axes (incl. color axis) = array elements
- Each dot = computation on some A(i), B(j), C(k)

- Optimization: Some blocking/tiling/ scheduling of this space



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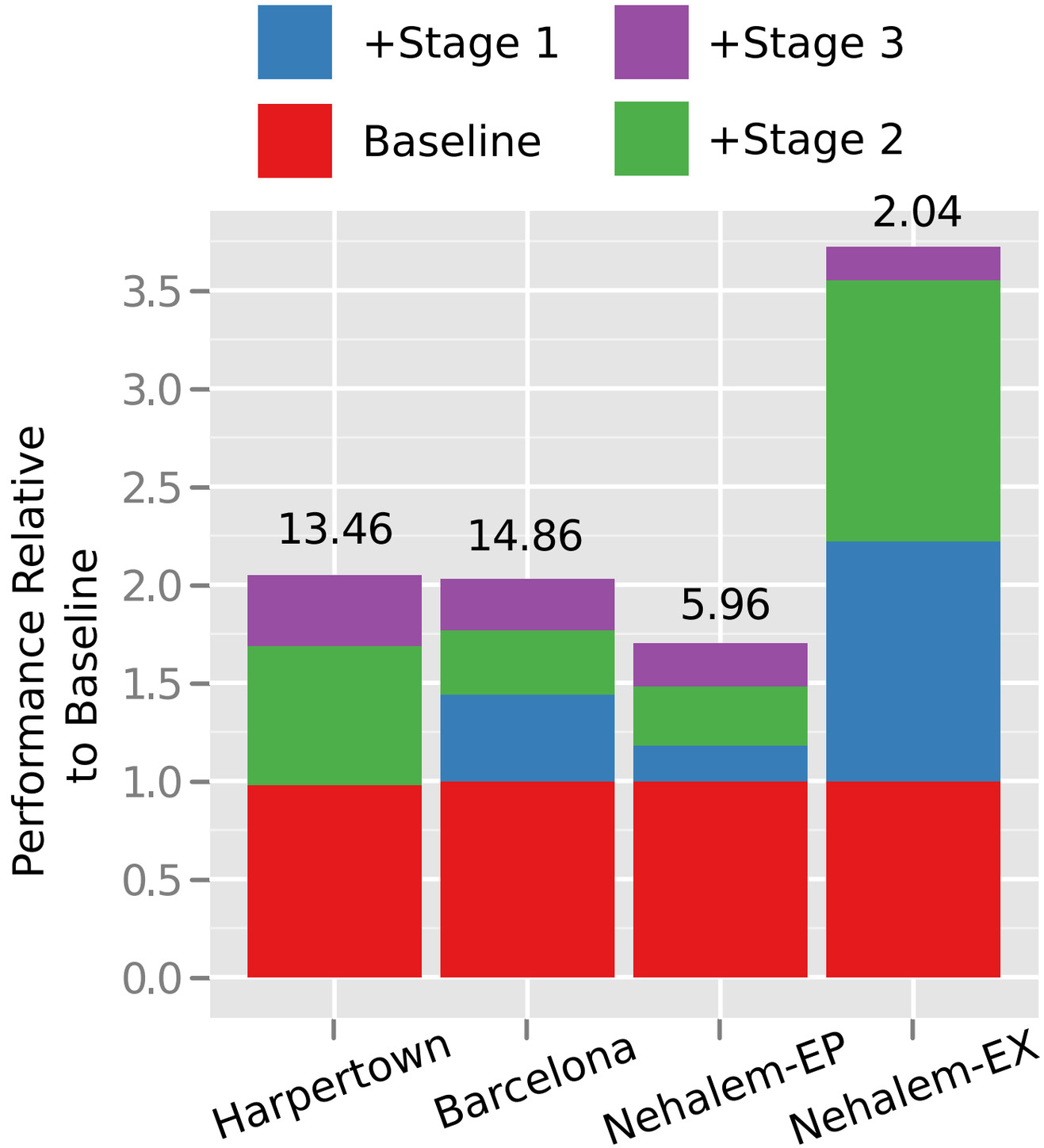

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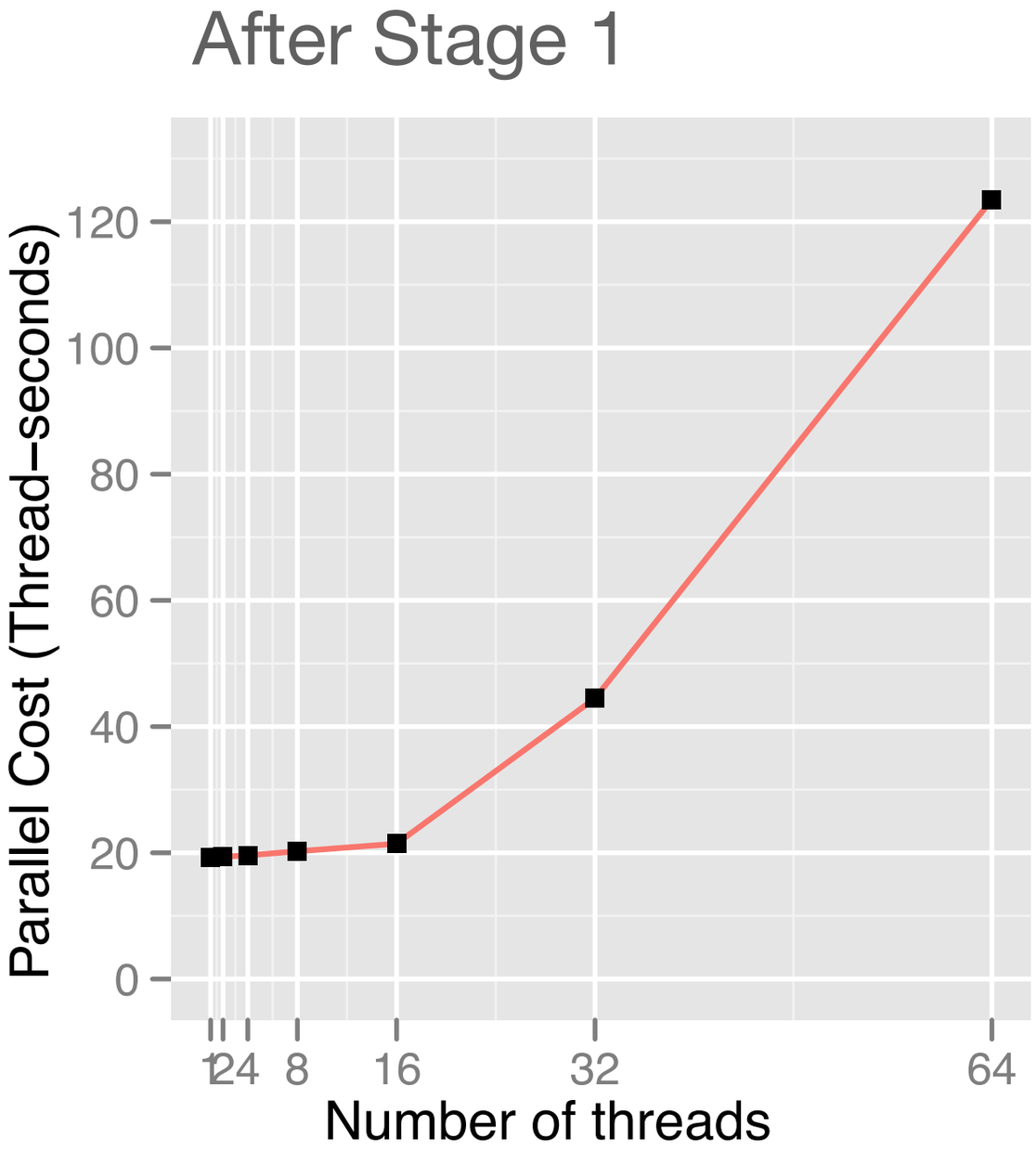
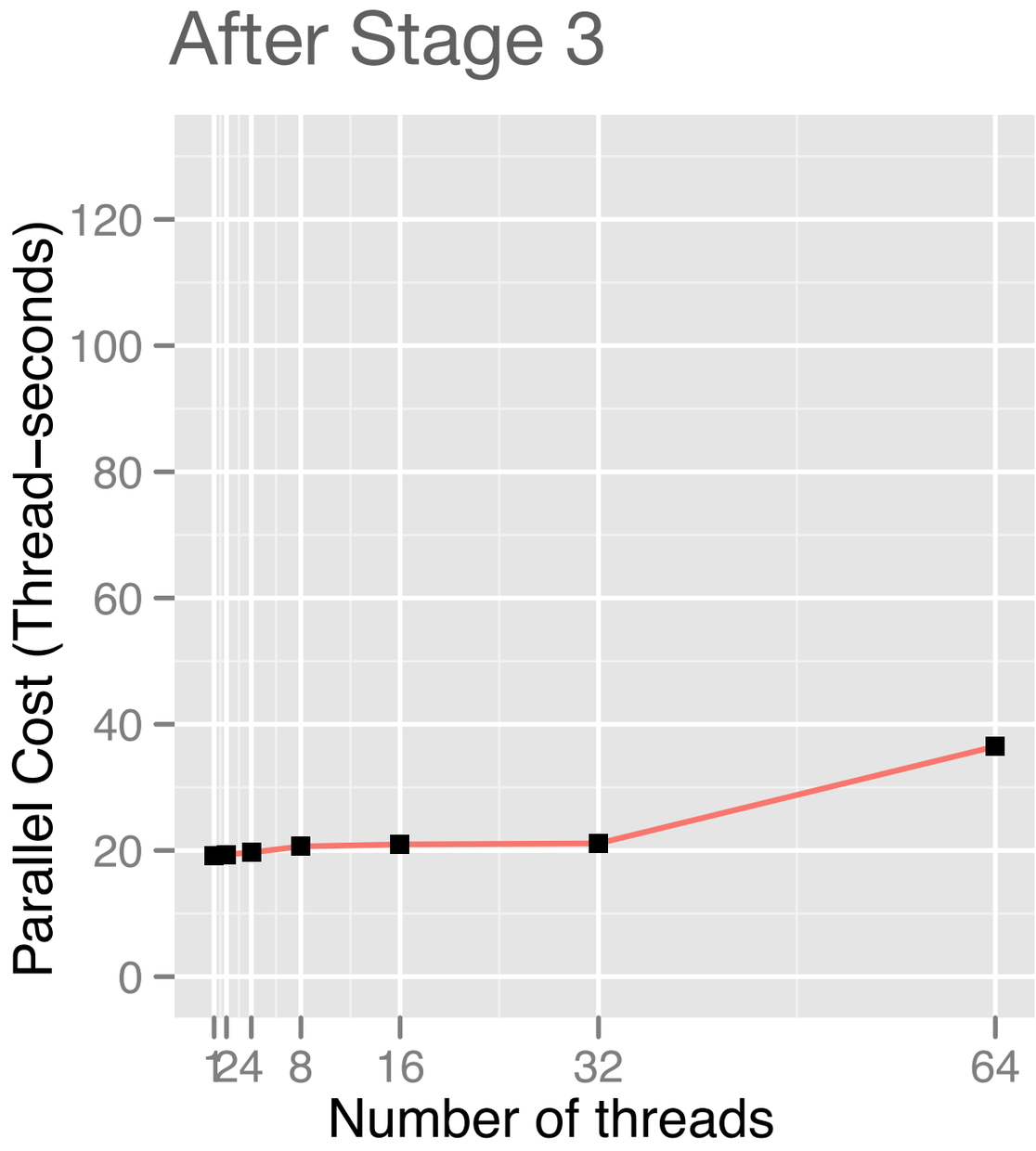
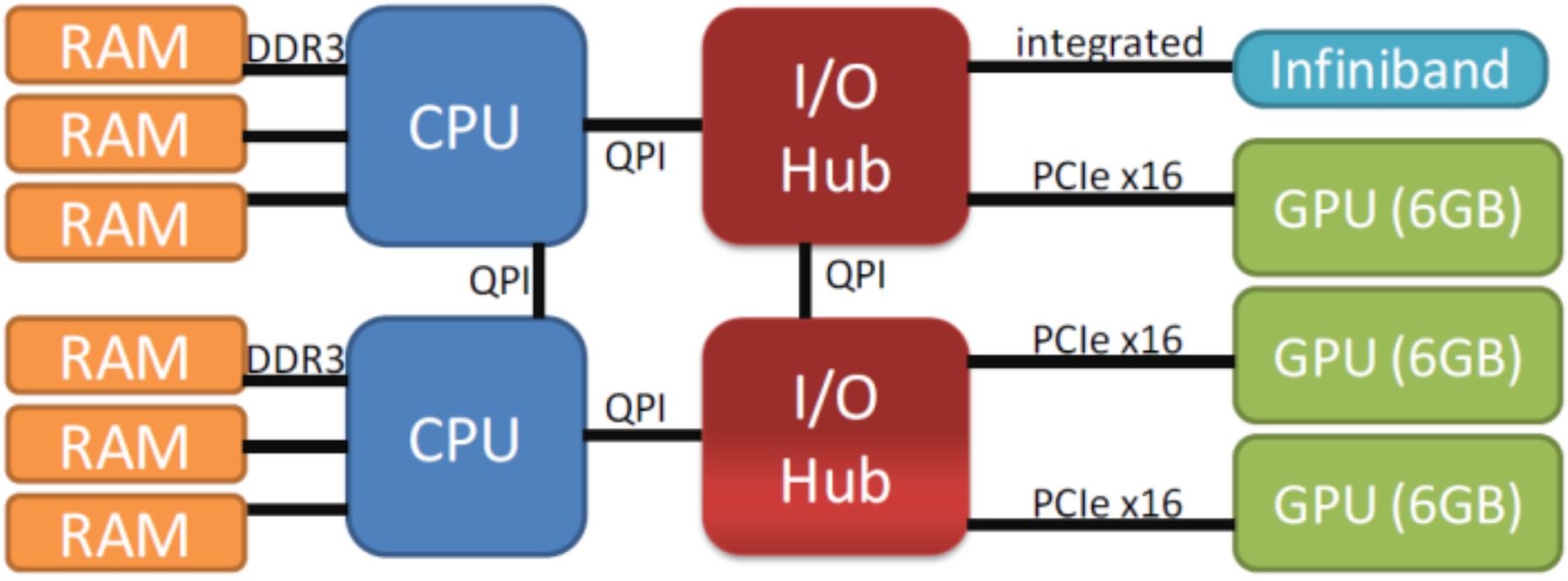
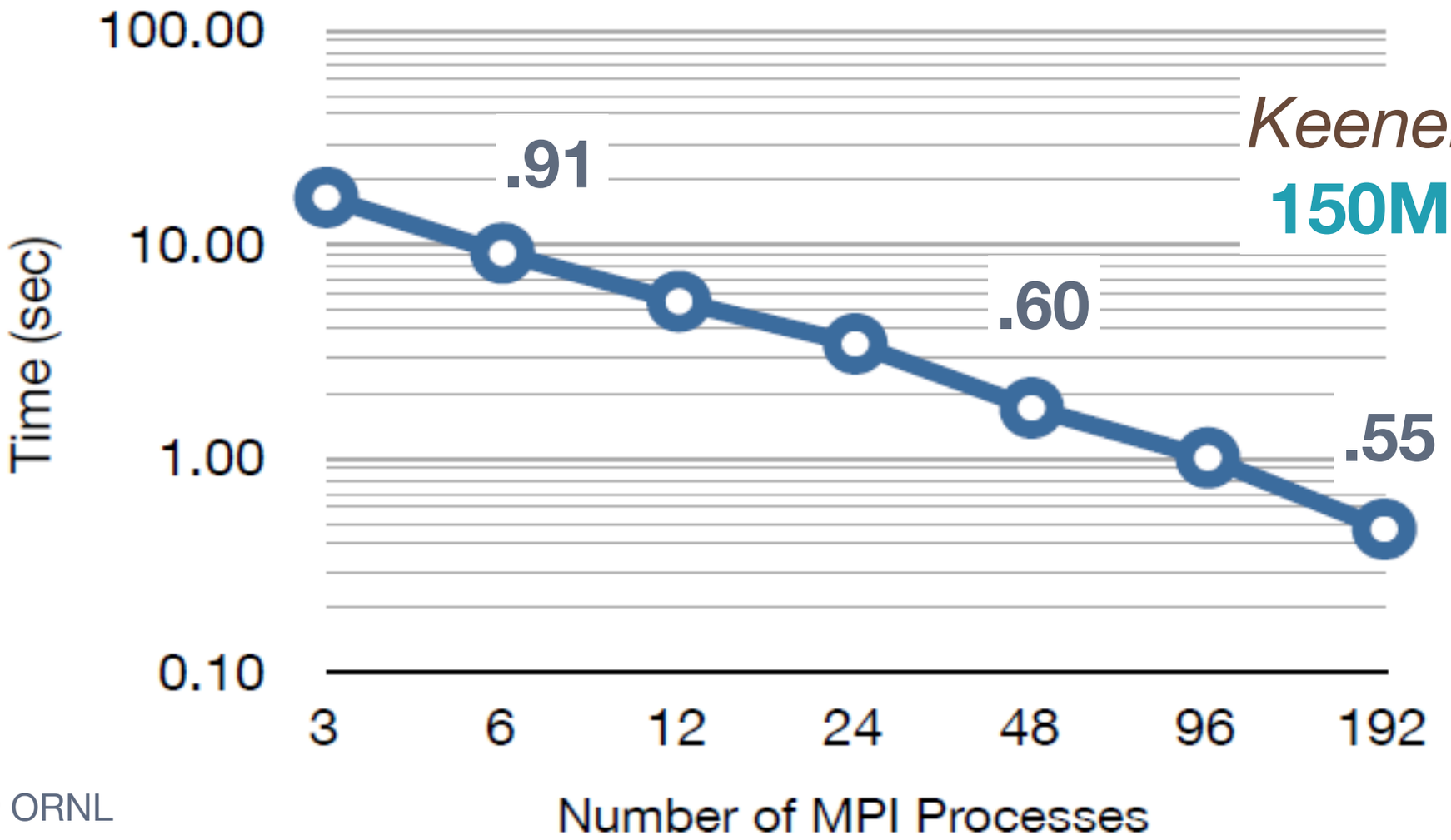




BEFORE & AFTER (NEHALEM-EX)

- Looking to exascale: Two cautionary predictions





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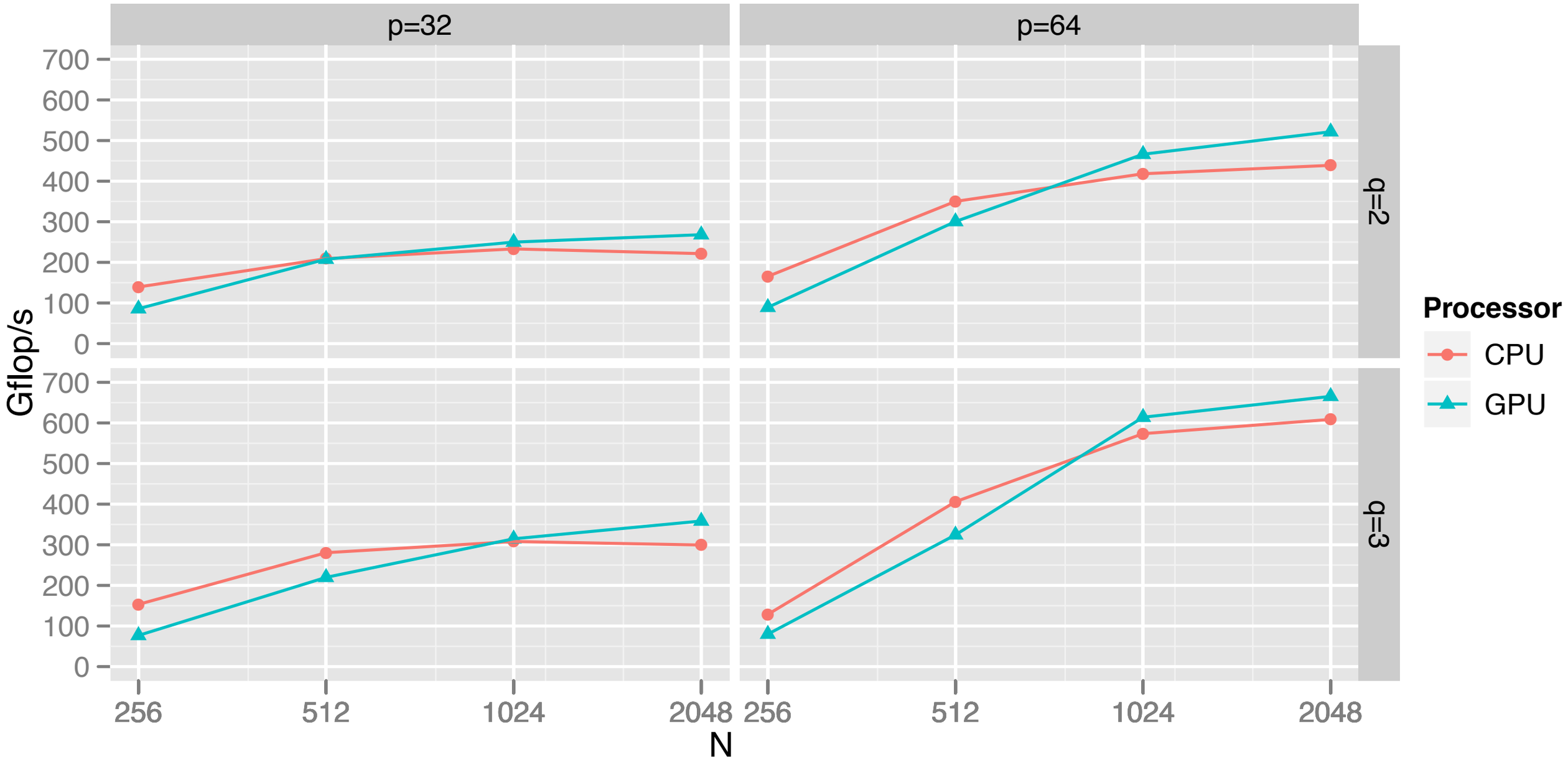
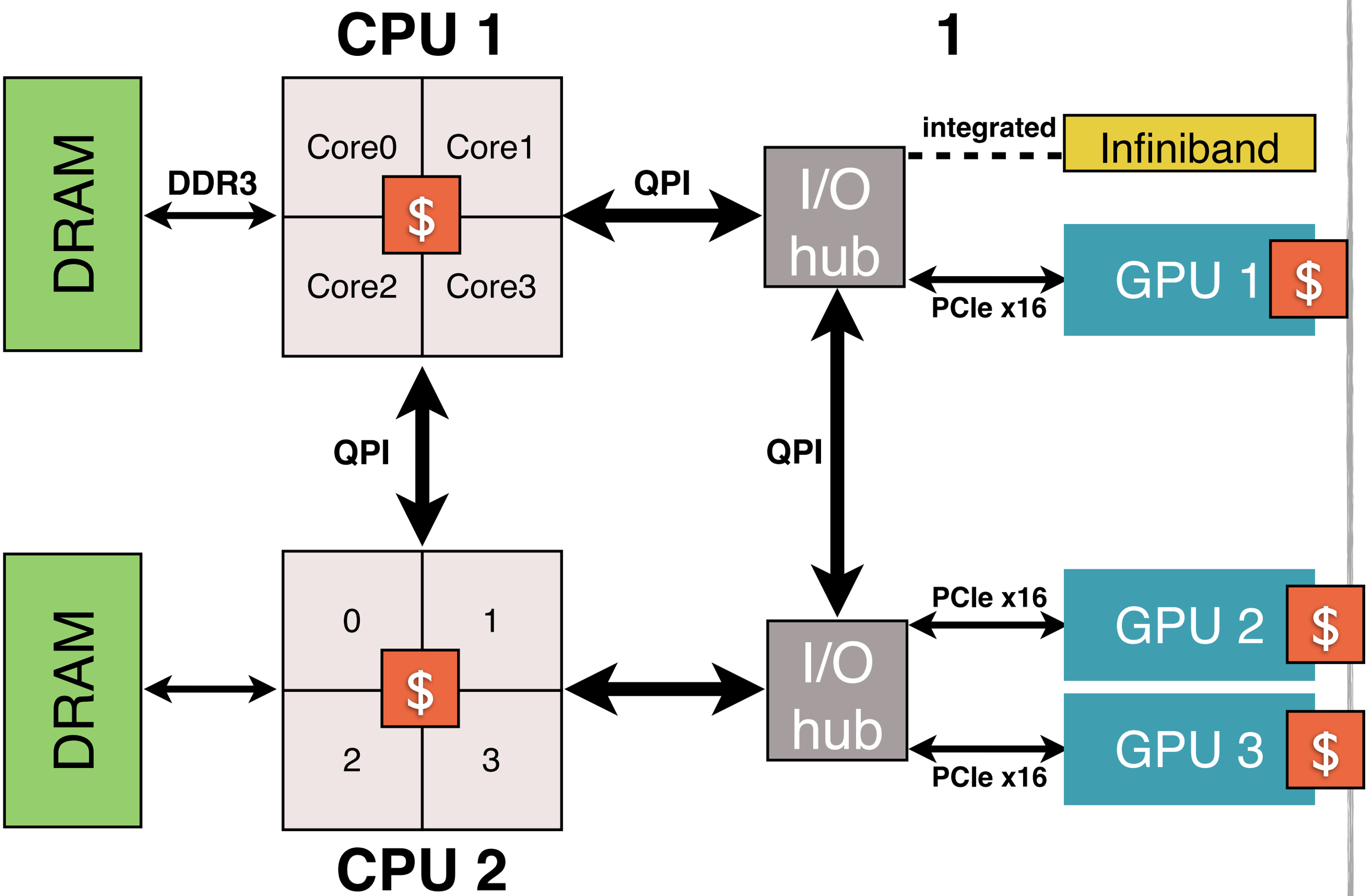
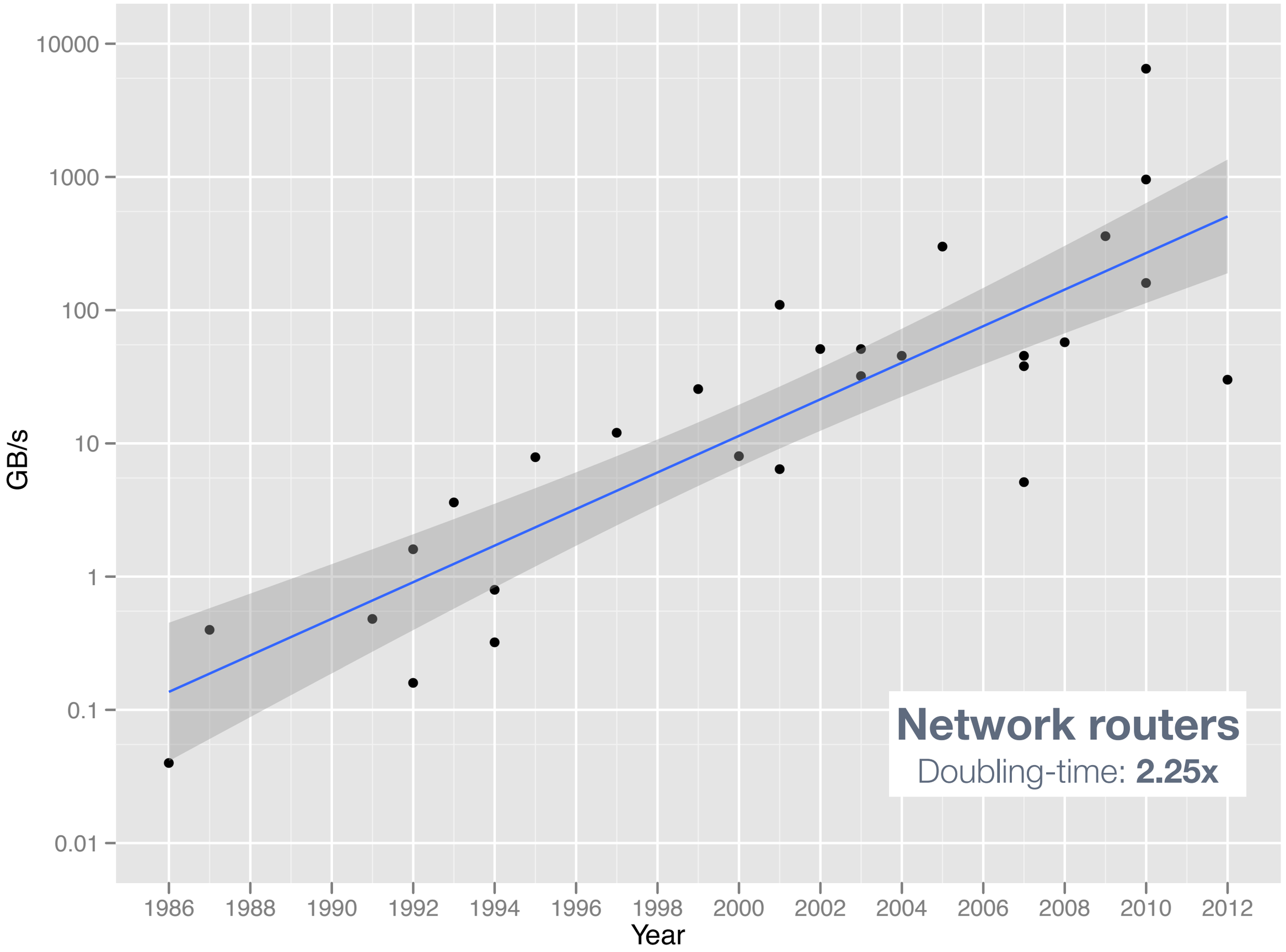
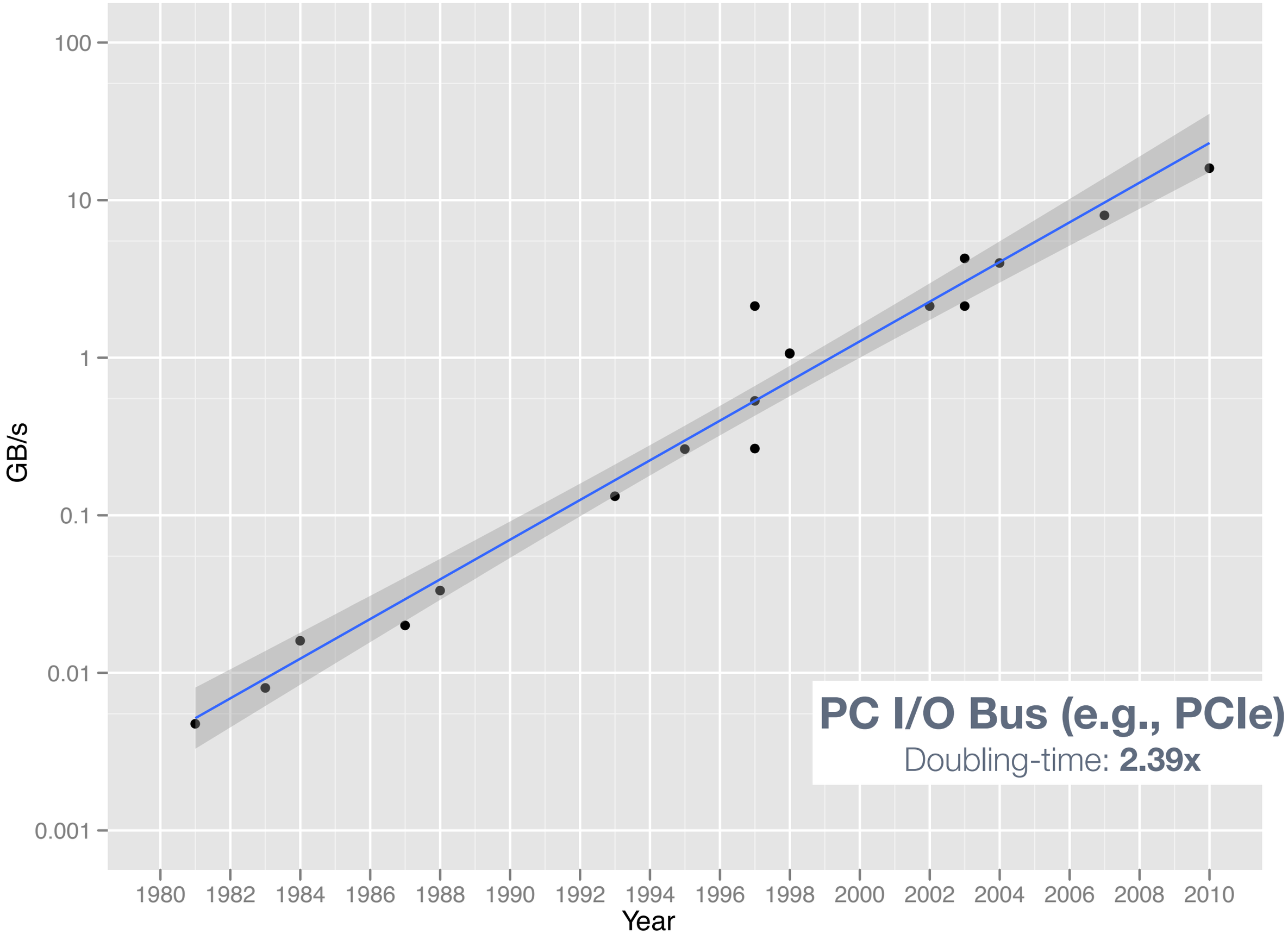


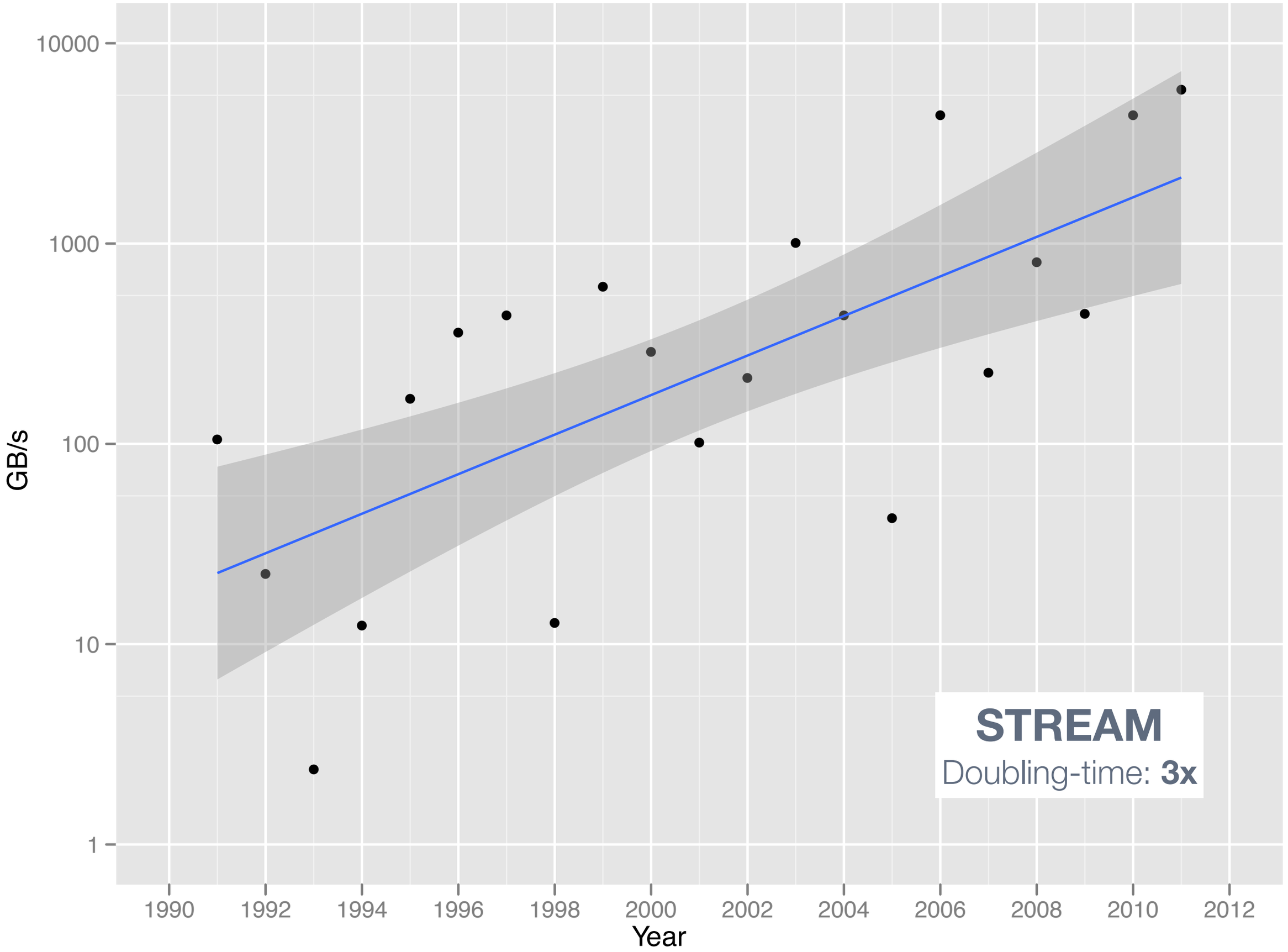
3D FFT, $N * N * N$ — P3DFFT, CUFFT vs. FFTW / MKL

Node


CPU 1
1
DRAM
DDR3
Core0
Core1
$
Core2
Core3
QPI
I/O hub
integrated
Infiniband
PCIe x16
GPU 1
$
QPI
PCIe x16
GPU 2
$
I/O hub
PCIe x16
GPU 3
$
DRAM
0
1
$
2
3
CPU 2


GB/s
10000
1000
100
10
1
0.1
0.01
1986
1988
1990
1992
1994
1996
1998
2000
2002
2004
2006
2008
2010
2012
Year
Network routers
Doubling-time: 2.25x


100
10
1
0.1
0.01
0.001
GB/s
1980
1982
1984
1986
1988
1990
1992
1994
1996
1998
2000
2002
2004
2006
2008
2010
Year
PC I/O Bus (e.g., PCIe)
Doubling-time: 2.39x


10000
1000
100
10
1
GB/s
1990
1992
1994
1996
1998
2000
2002
2004
2006
2008
2010
2012
Year
STREAM
Doubling-time: 3x

3D FFT Swim Lanes: A prediction for 2020