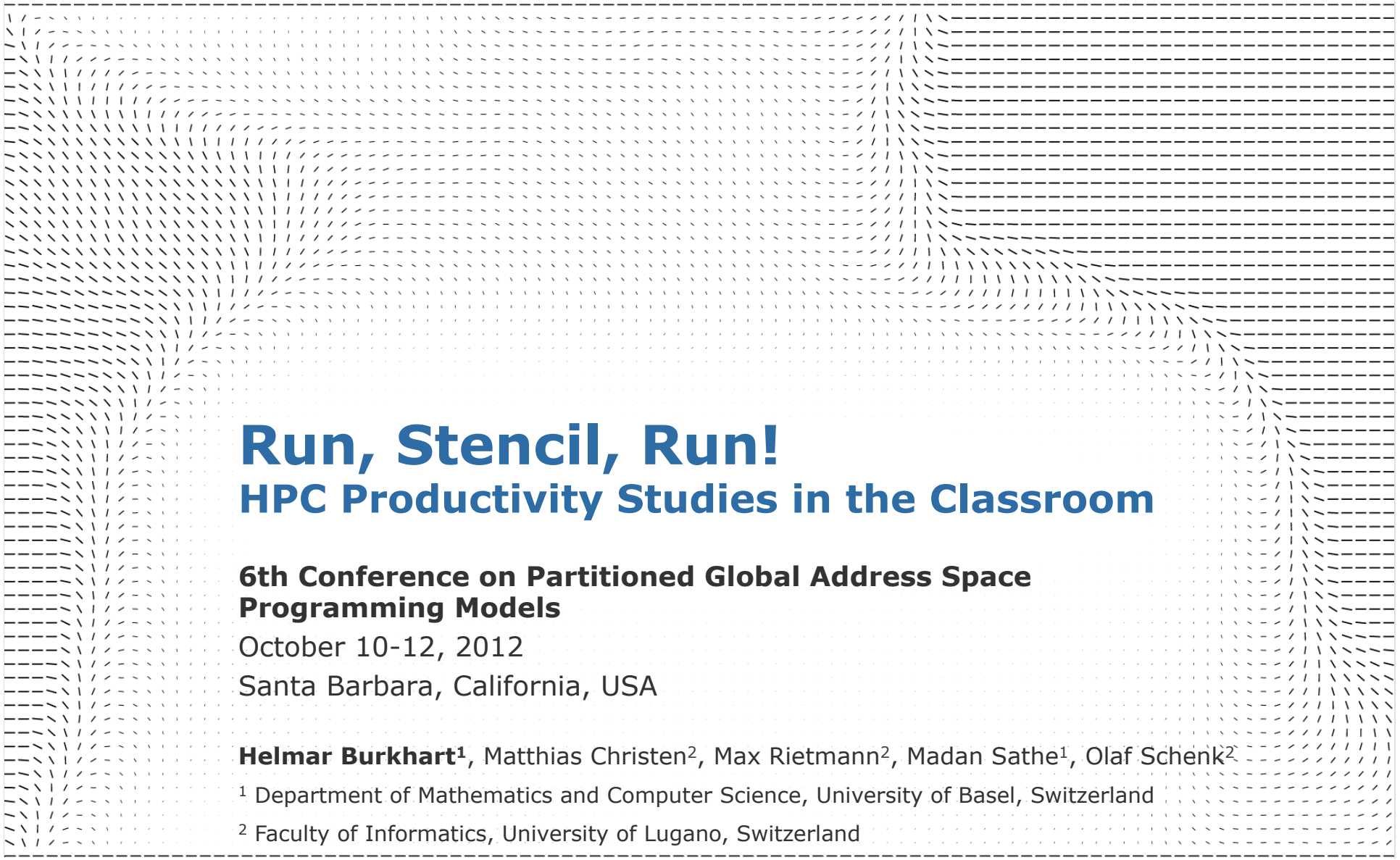
University of Basel



Run, Stencil, Run!

HPC Productivity Studies in the Classroom

6th Conference on Partitioned Global Address Space Programming Models

October 10-12, 2012

Santa Barbara, California, USA

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UNI BASEL

P-Challenges 2012 and Beyond

- **P**erformance: Preparations for Exascale.
- **P**ower: Computation cheap, data movement expensive.
- **P**arallelism: > 10^6 fine-granular schedules.
- **P**rogrammability: GPLs & DSLs, Libraries.
- **P**ortability: Late System-binding. Auto-tuning.

- **P**roductivity: What is it? How to measure?

Where to Find a Crowd for Productivity Studies?

- Do **not** want **experienced HPC programmers** who have already personal favourites.

  ⟶ Newcomers open to all parallel programming models.

- Do **not** want **pure HPC enthusiasts.**

  ⟶ Good mix of users: Some freaks, but majority wants to do just their job.

MSc students in Computer Science are a reasonable approximation for such a crowd!

Before my course!

Part I: Classroom Studies

CS311 High-Performance Computing

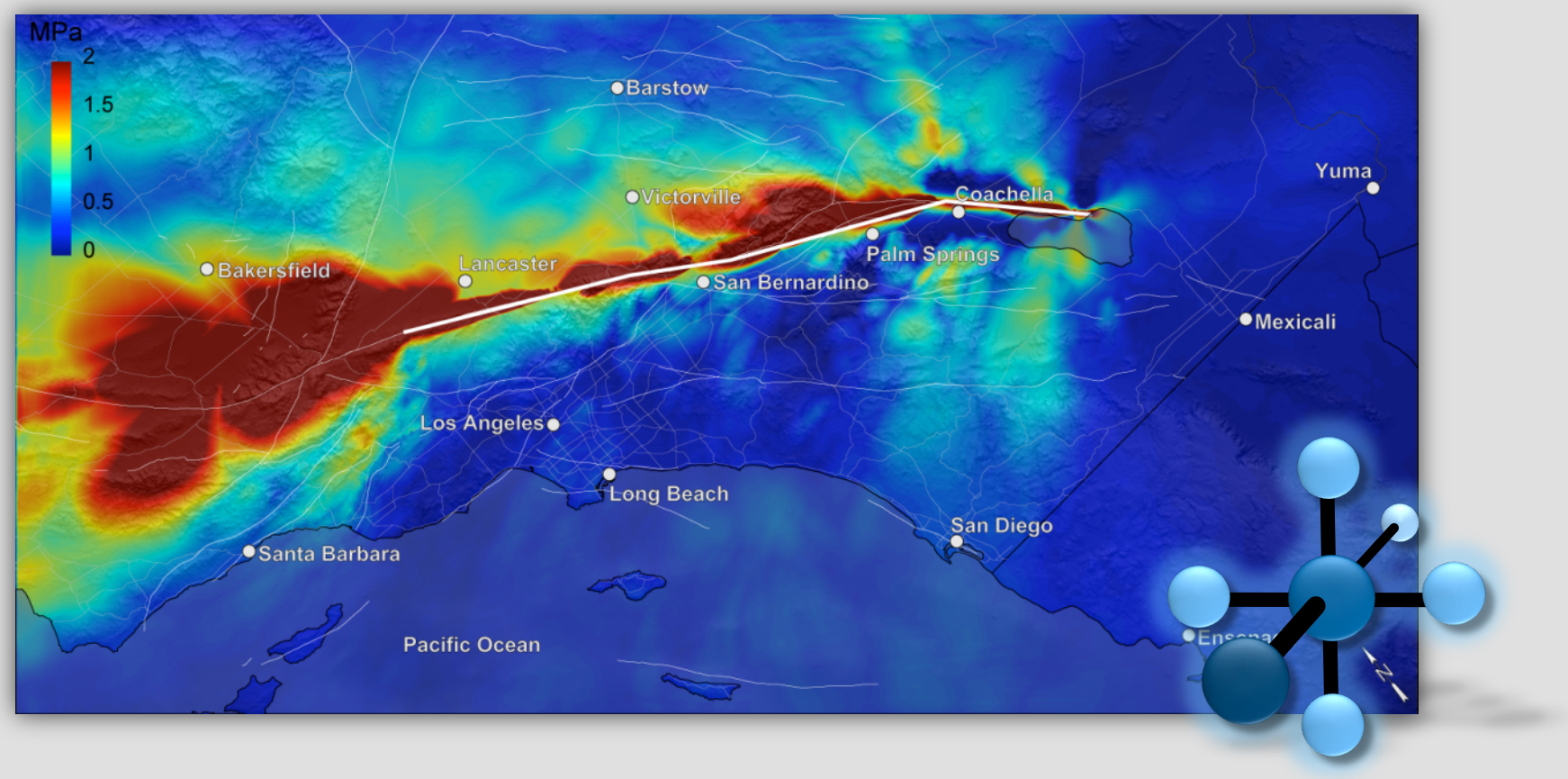
- Lectures: Algorithms, Architecture, and **Programming**
- Lab work mandatory
- 6 ECTS Credit points (=180h work).

Audience

- Graduate-level course
- Computer Science and Computational Science master students, a few PhD students.
- 15 participants in 2012

Challenge: How do make students familiar **both** with **state-of-the-art and next-generation HPC**?

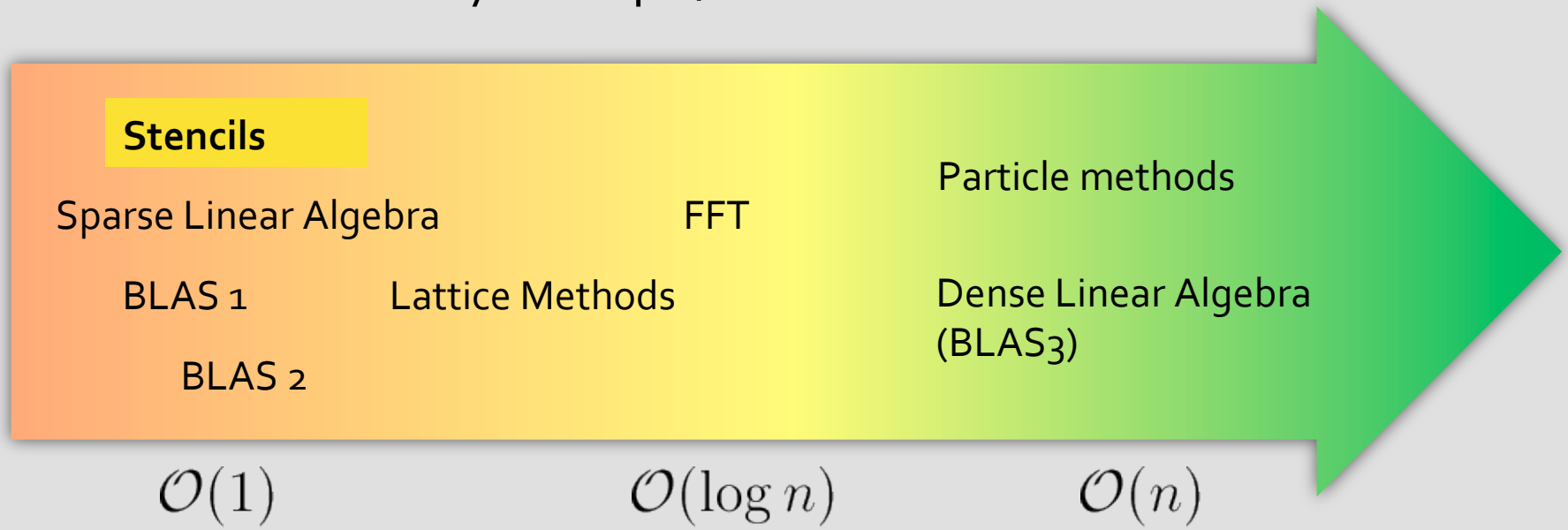
Stencil Motif is Motivating



- Geo-Physics
- Meteorology
- Computational Medicine
- Engineering
- Image Processing
- …

Stencil Motif is a Challenge

Arithmetic Intensity := Flops / Transferred Data



Low arithmetic intensity
⇒ memory bandwidth bound

High arithmetic intensity
⇒ processor bound

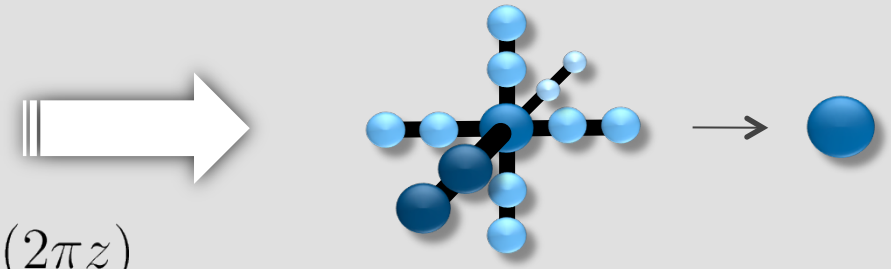
Students' Problem to be Solved

Solve the classical wave equation using finite differences.

$$\frac{\partial^2 u}{\partial t^2} - c^2 \nabla^2 u = 0 \qquad \text{in } \Omega$$

$$u \equiv 0 \qquad \text{on } \partial\Omega$$

$$u(x, y, z, 0) = \sin(2\pi x)\sin(2\pi y)\sin(2\pi z)$$



Pseudo-code and Experiment Settings

Algorithm 1 Pseudo-code for the iterative stencil computation

Require: Arrays u^-, u^0; Stencil operator ∇_h^2
Ensure: Array u^+

1: **for** $t \leftarrow 1 \ldots t_{\max}$ **do** ▷ *Iterate over the time domain*
2: ▷ *Iterate over the discrete domain, the index set* Ω_h
3: **for** $(i, j, k) \in \Omega_h$ **do**
4: ▷ *Compute the next time step at* (i, j, k)
5: $u^+_{ijk} \leftarrow 2u^0_{ijk} - u^-_{ijk} + \Delta t^2 c^2 \nabla_h^2 u^0_{ijk}$
6: **end for**
7: $u^- \leftarrow u^0$; $u^0 \leftarrow u^+$ ▷ *Rotate arrays (copy semantics)*
8: **end for**

Parameter Settings:

- 200^3 grid points
- 19 Flops per grid point
- 100 time steps

Target 1: CPU System

- 4 quad-core Intel Xeon E7420 (“Dunnington”) CPUs, 2.1 GHz
- 32 KB L1 data cache
- 3 MB unified L2 cache, shared among 2 cores
- 8 MB L3 cache, shared among 4 cores
- 128 GB DDR3 RAM
- 8.3 GB/s BW (measured)

Target 2: GPU System

- 14 "streaming multiprocessors", 448 CUDA cores, 1.15 GHz
- 64 KB shared memory per streaming multiprocessor
- 3 GB GDDR5 RAM
- 79 GB/s BW (measured)

Programming Models to Explore

- Java Concurrency

Mainstream language going parallel

- Chapel
- PATUS

New high-level GPL & DSL

- OpenMP
- MPI
- CUDA

State-of-the-art industry use

Java Excerpt (Part 1)

```
class Calculator implements Runnable {
private int m_nStart;
private int m_nEnd;

public Calculator(int nStart, int nEnd) {
   m_nStart = nStart; m_nEnd = nEnd;
}

@Override public void run() {
for (int k = m_nStart; k < m_nEnd; k++)
  for (int j = 2; j < y_max - 2; j++)
    for (int i = 2; i < x_max - 2; i++)
       u_1[k][j][i]=2*u_0[k][j][i]-u_m1[k][j][i]+...
}
}
```

Class & Interface

Constructor

Method overwrite

Java Excerpt (Part 2)

```
public static void main (String[] args) {
final int nNumThreads =  Runtime.getRuntime().availableProcessors();
final ExecutorService executor =
  Executors.newFixedThreadPool(nNumThreads);
final int nPlanesPerThread = (z_max-4) / nNumThreads;

for (int t = 0; t < t_max; t++) {
  List<Future<?>> listFutures = new ArrayList<>();
  // submit parallel tasks
  for (int i = 0; i < nNumThreads; i++)
    listFutures.add(executor.submit(
      new Calculator(i*nPlanesPerThread+2, (i+1)*nPlanesPerThread+2)));
  for (Future<?> future : listFutures) { // synchronize
    try { future.get (); } catch ... }
  float[][][] tmp = u_m1; u_m1 = u_0; u_0 = u_1; u_1 = tmp;  }
executor.shutdown();
```

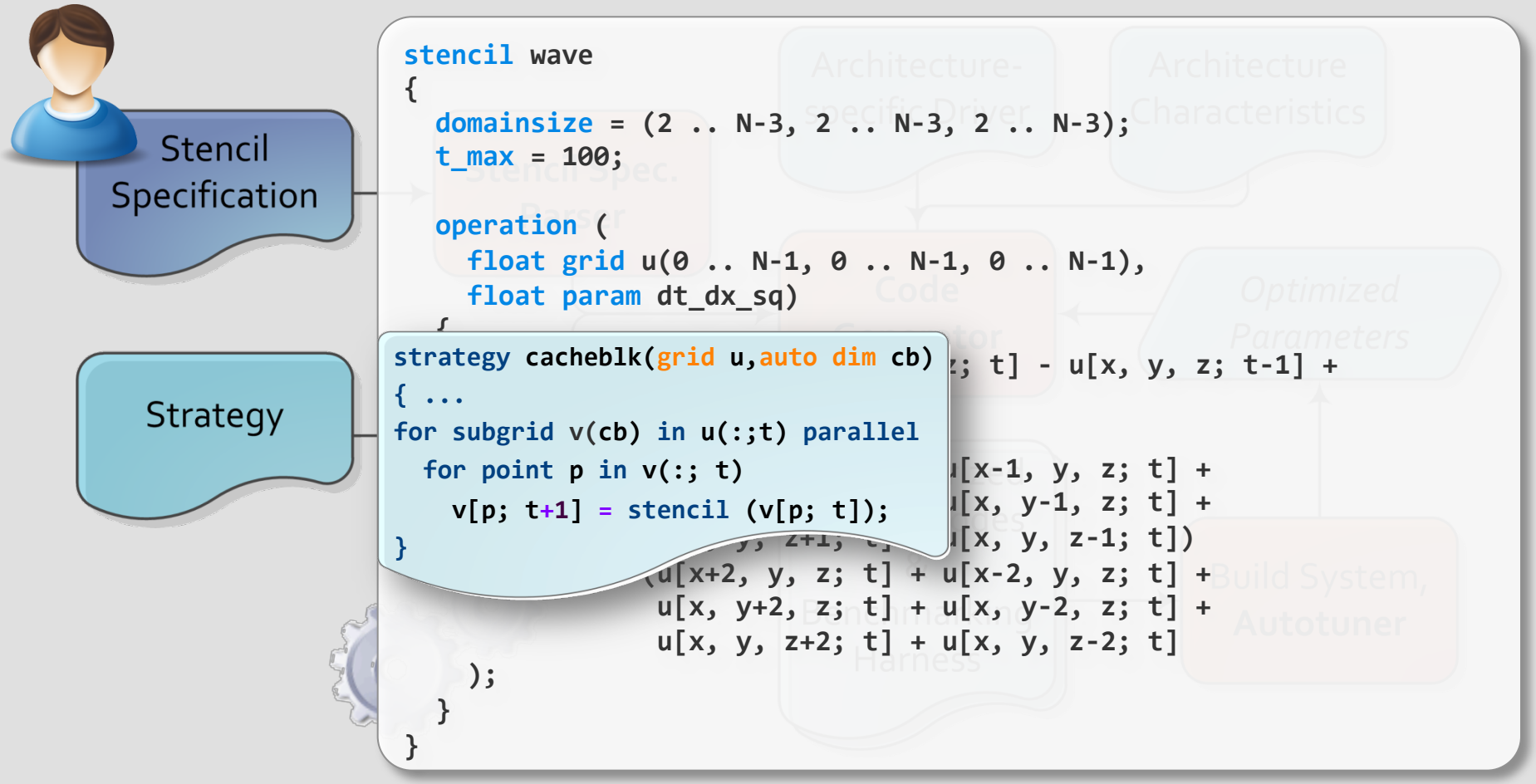
Execution framework

High-level structures for asynchroneous thread control

Concurrent data structures

Data partitioning and distribution missing

PATUS: Parallel Auto-Tuned Stencils



M. Christen, O. Schenk, and H. Burkhart, *PATUS: A Code Generation and Autotuning Framework For Parallel Iterative Stencil Computations on Modern Microarchitectures*, IPDPS 2011

Questionnaire

#Threads	Time [seconds]	GFlop/s	Speedup	Efficiency
1				
2				
4				
8				
16				

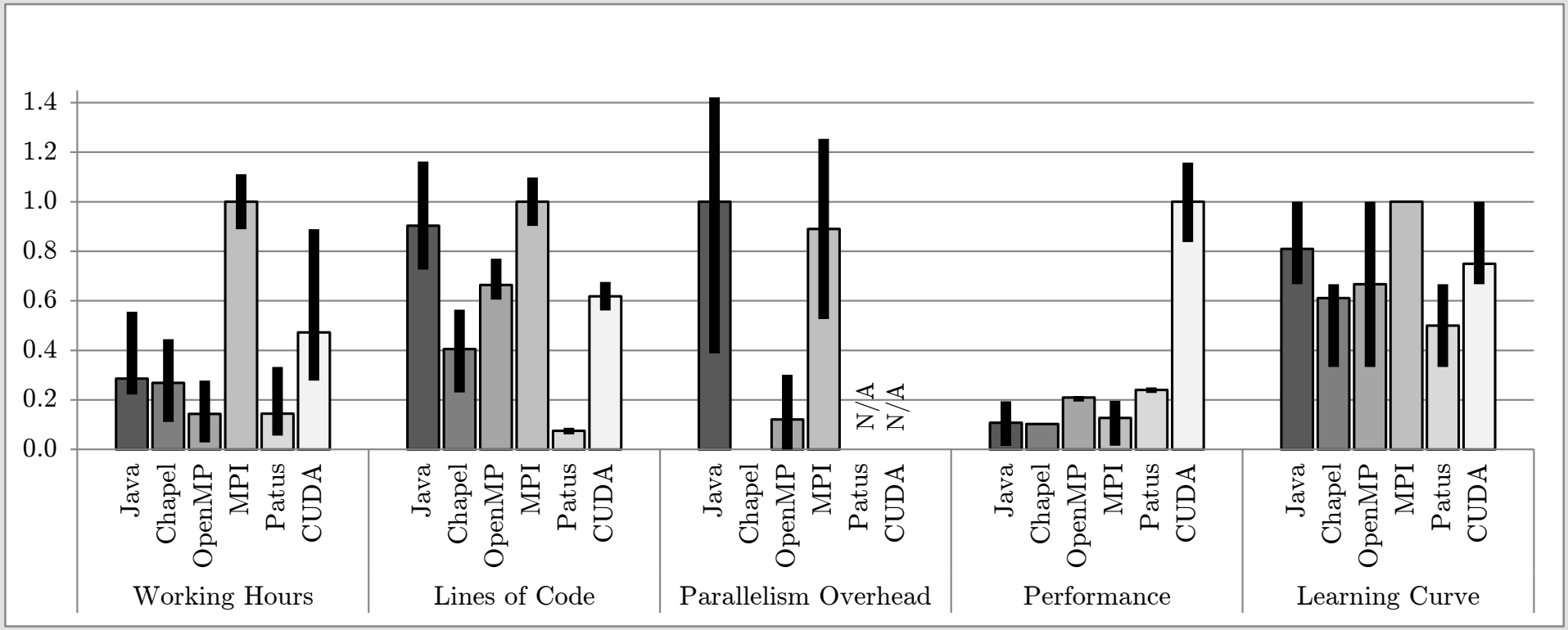
Productivity:

- Time spent on parallelization: ☐ hours
- Lines of source code: sequential: ☐ parallel: ☐
- Learning curve: ◯ easy ◯ medium ◯ hard
- Difficulties during programming:
  - Source of errors (index calculation, parallelization, …)

    ☐
  - Kind of errors (conceptional understanding, syntax, programming, ...)

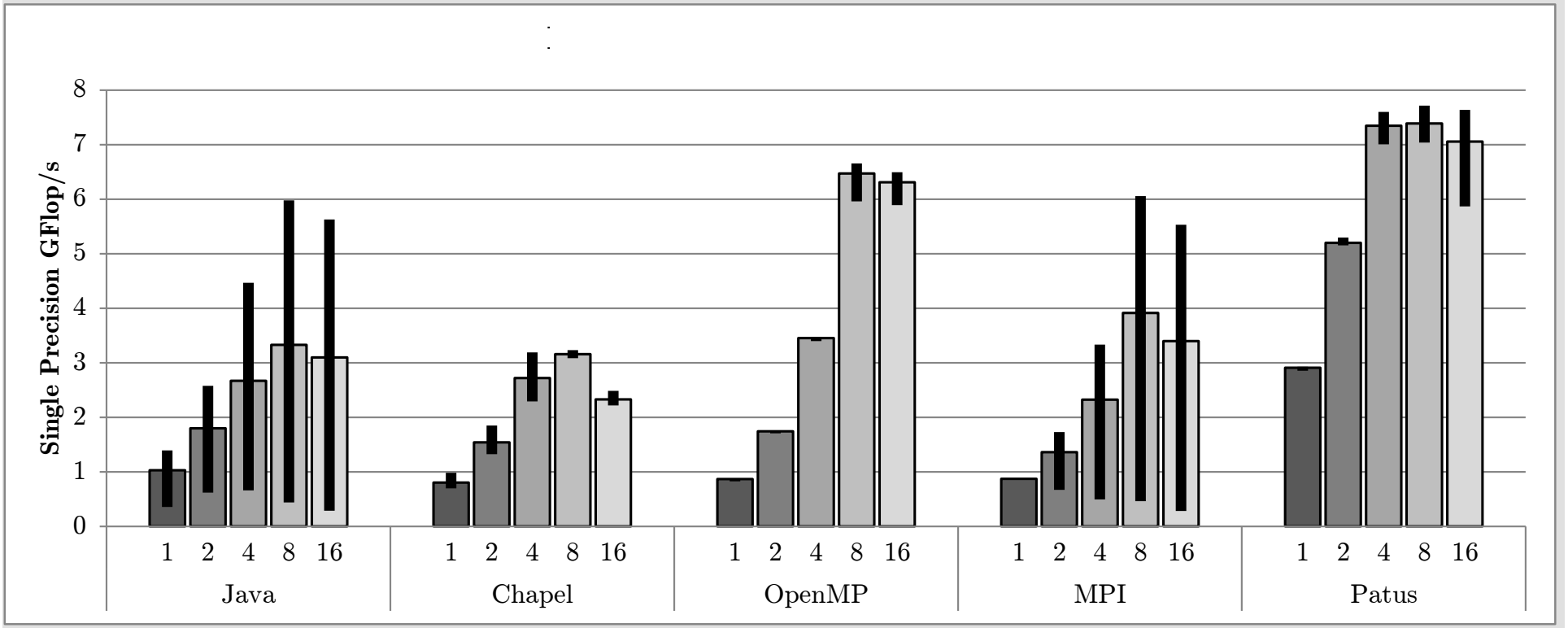
    ☐

Data Collected from Questionnaires

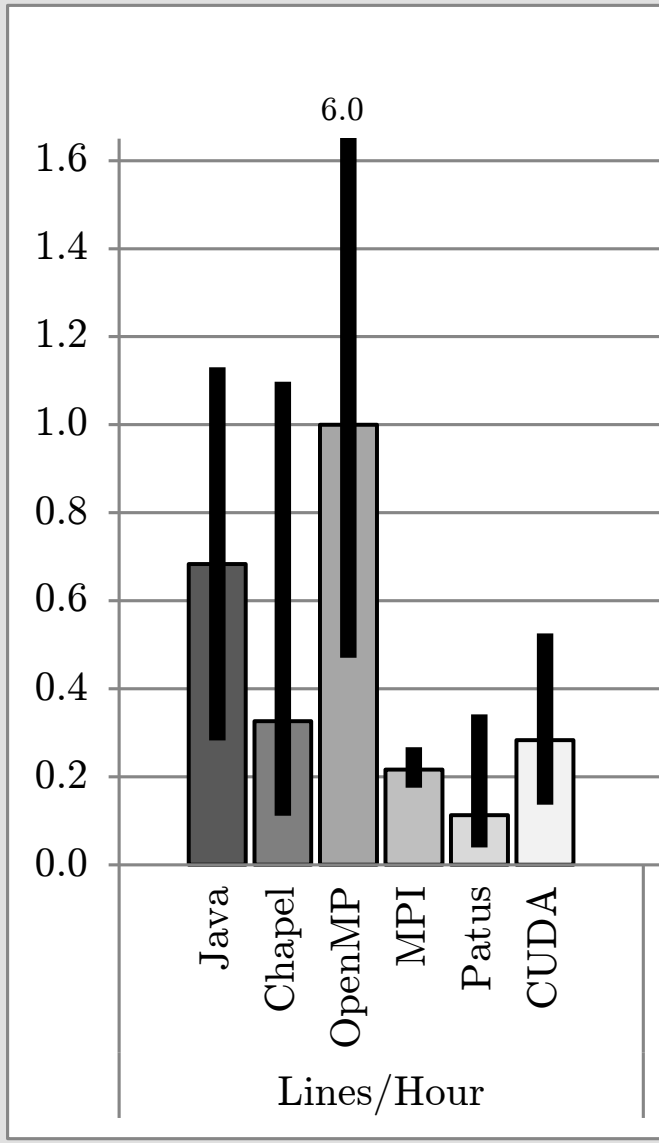


Programming Model	Working Hours	Parallel Overhead	Best Performance [GFlop/s]	Lines of Code	Learning Curve [1≙easy, 3≙hard]
Java	5.14	35%	5.98	267	2.4
Chapel	4.83	0%	3.23	120	1.8
OpenMP	2.58	4%	6.66	197	2.0
MPI	18.00	32%	6.06	296	3.0
PATUS	2.60	*N/A*	7.72	22	1.5
CUDA	8.50	*N/A*	35.70	183	2.25

Performance Benchmark



Productivity (1)



?

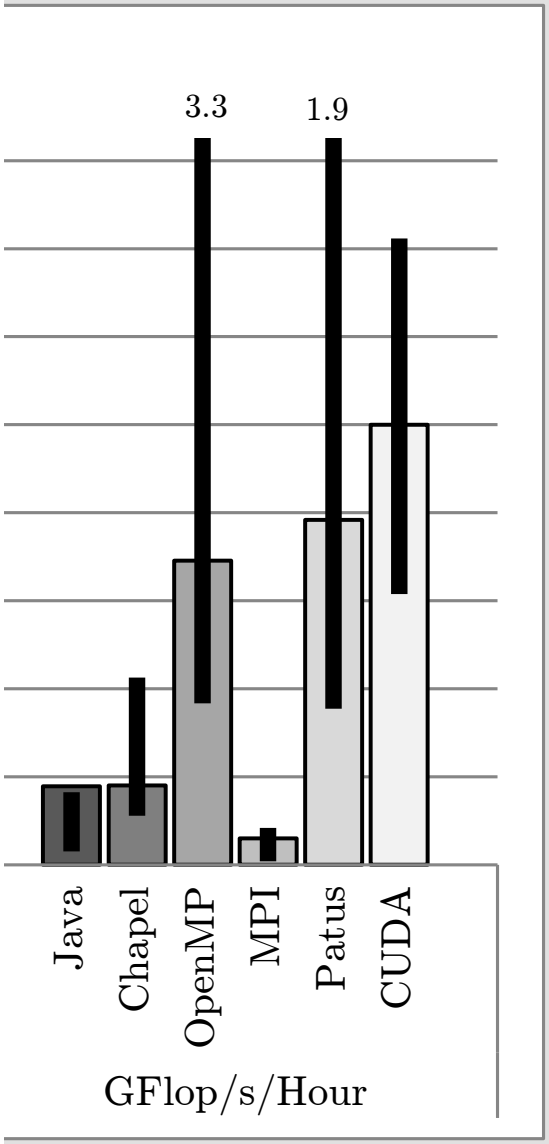
Coding Productivity =

Lines of Code / Working hours

Productivity (2)

Performance Productivity =

Performance Achieved / Working hours



Part II: Post-Classroom PGAS Experiments

- How do different PGAS languages compare?
- What performance gain is achievable by hand-made PGAS program tuning?
- Same problem, same target system.
- Advanced HPC programmers / language implementors may find more optimization parts!

Chapel 1: Domain Shifting

```
const
  Domain = [ 0..x_max-1, 0..y_max-1, 0..z_max-1 ],
  Inner = Domain.expand(-2),
  Left1 = Inner.translate(-1, 0, 0),
  Right1 = Inner.translate(1, 0, 0), ...
var u_m1, u_0, u_1: [ Domain ] real(32);
for t in 1 .. t_max {
  u_1[Inner] = c1 * u_0[Inner] - u_m1[Inner] +
    dt_dx_sq * (
      c2 * u_0[Inner] +
      c3 * (u_0[Left1] + u_0[Right1] + u_0[Back1] + ...) -
      c4 * (u_0[Left2] + u_0[Right2] + u_0[Back2] + ...));
  u_m1 = u_0; u_0 = u_1;
}
```

Chapel 2: Subdomain and Reduction

```
const Stencil: sparse subdomain([-2..2, -2..2, -2..2]) = (
  (0,0,0), (-2,0,0), (-1,0,0), (1,0,0), (2,0,0), ...);
var c: [ Stencil ] real(32);
c[(0, 0, 0)] = c1; c[(-1, 0, 0)] = c2; ...
for t in 1 .. t_max {
  forall i in Inner do
    u_1(i)=(+ reduce [j in Stencil] c(j)*u_0(i+j))-u_m1(i);
  u_m1 = u_0; u_0 = u_1;
}
```

Chapel 3: Domain Map

```
const
  Domain: domain(3) dmapped Block (
    boundingBox = [0..x_max-1,0..y_max-1,0..z_max-1]) =
    [ 0..x_max-1, 0..y_max-1, 0..z_max-1 ],
  Inner: domain(3) dmapped Block (
    boundingBox = [0..x_max-1,0..y_max-1,0..z_max-1]) =
    Domain.expand(-2);
```

Chapel 4: Nested Loops

```
for t in 1 .. t_max {
  forall z in 2 .. z_max-3 do
    for y in 2 .. y_max-3 do
      for x in 2 .. x_max-3 do
        u_1(x,y,z) = c1 * u_0(x,y,z) - u_m1(x,y,z) +
          dt_dx_sq * (c2 * u_0(x,y,z) +
            c3 * (u_0(x+1,y,z) + u_0(x-1,y,z) + ...));
  u_m1 = u_0; u_0 = u_1;
}
```

Chapel 5: Zippered Iterator

```
for t in 1 .. t_max {
  forall (x,y,z) in Inner do
    u_1(x,y,z) = c1 * u_0(x,y,z) - u_m1(x,y,z) + ...
  u_m1 = u_0; u_0 = u_1;
}
```

Chapel 6: 4D-Grid

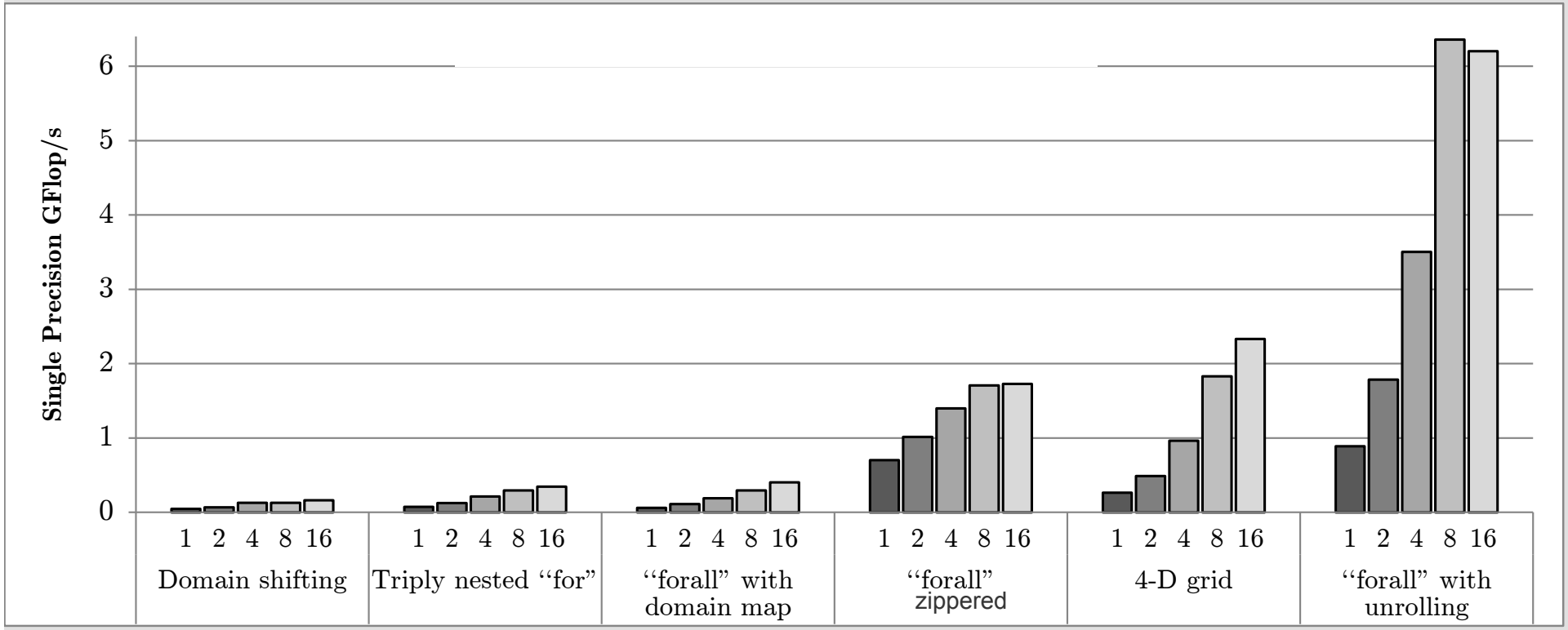
```
const
  Inner = [ 1..x_max, 1..y_max, 1..z_max, 0..2 ],
  Domain = DomainInner.expand (2, 2, 2, 0);
var u: [ Domain ] real(32);
for t in 1 .. t_max {
  forall (x,y,z) in Inner do

    u(x,y,z,t_1) = c1 * u(x,y,z,t_0) - u(x,y,z,t_m1) + ...
  t_1 += 1;  if (t_1 > 2) then t_1 -= 3; // etc. (t_0, t_m1)
}
```

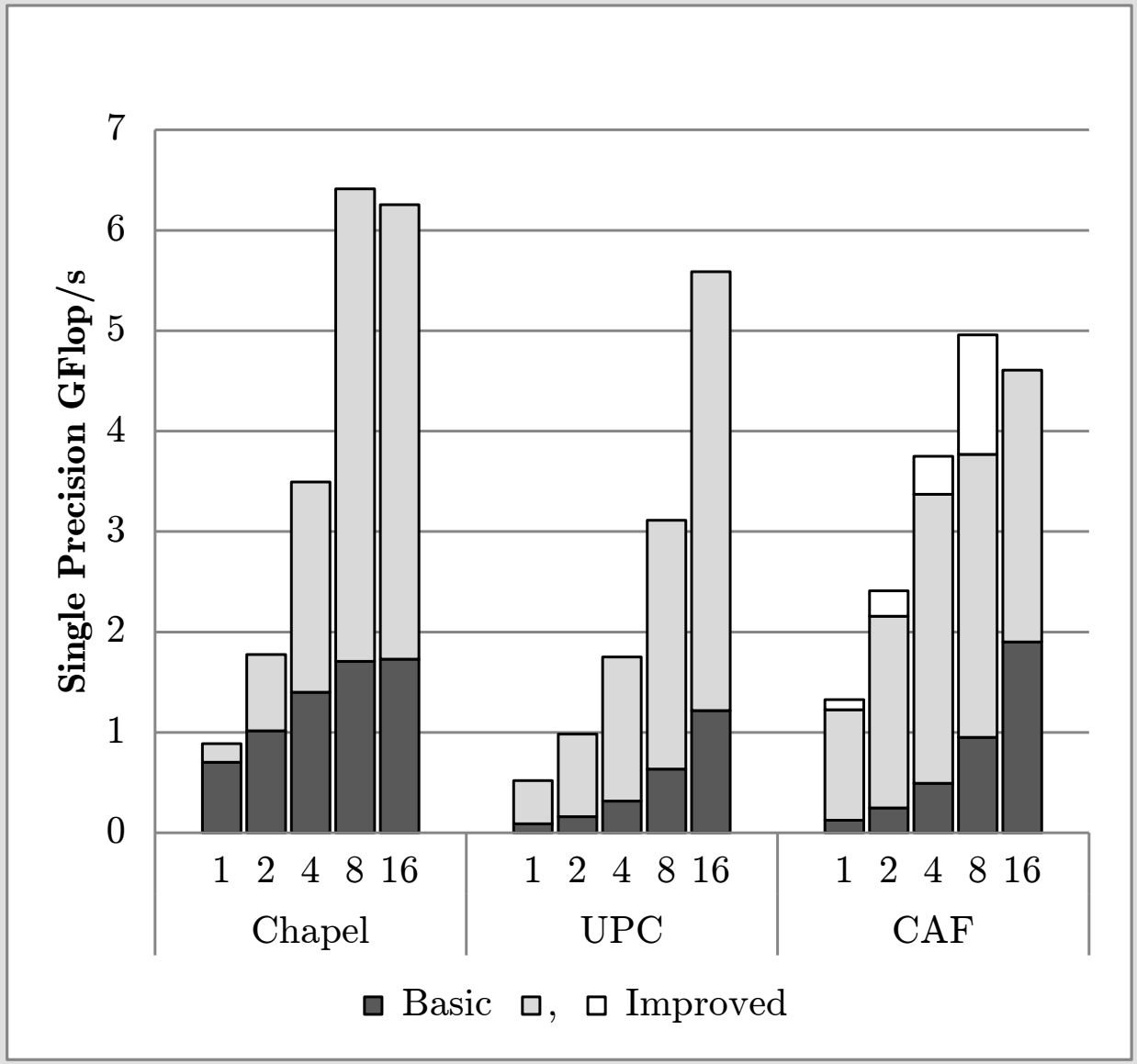
Chapel 7: Loop Unroll

```
for t in 1 .. t_max/3 {
  forall (x,y,z) in Inner do
    u_1(x,y,z) = c1 * u_0(x,y,z) - u_m1(x,y,z) + ...
  forall (x,y,z) in Inner do
    u_m1(x,y,z) = c1 * u_1(x,y,z) - u_0(x,y,z) + ...
  forall (x,y,z) in Inner do
    u_0(x,y,z) = c1 * u_m1(x,y,z) - u_1(x,y,z) + ...
}
```

Chapel Performance for Variants



PGAS Language Comparisons



Conclusions

- As parallel processing goes mainstream, **enhanced *productivity benchmarks* are needed**.
- Our studies show that **PGAS languages already do quite well** compared to production models (with much longer history).
- Multi-resolution approach like in Chapel is good for algorithmic creativity but ***cost models* are needed** to predict performance at early stages.
- **Performance tuning within the PGAS domain is possible.**It is up to the time and money budget how far you go.
- **PGAS is the right approach for HPC education**.

Outlook

Run, Stencil, Run will be continued, a new crowd is waiting:

- Multinode target system
- X10 experiments
- …

All suggestions how to get improved studies are highly welcome

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