Main Seminar
Hot Topics in Bioinformatics

Alexandros Stamatakis

Now

- **How to give a scientific presentation**
- How to write a technical report/scientific paper

Scientific Presentations

- This is my personal view, based on over 120 talks I have given
- At CS conferences: typically 25 minutes + 5 minutes questions
- Timing
  - Practice your talk beforehand
  - Usually 1.5-2 minutes per slide
  - Keep in mind, when presenting one usually talks faster than during the rehearsal
  - Use SW tools for timing, e.g., sliding time bars
  - Use a **spell-checker** for the slides!

The audience

- Giving talks gets easier and easier the more talks you give
- Try to imagine what kind of audience you might be expecting
- What may or may they not know about the problem at hand?
- What terms & acronyms can be assumed to be standard knowledge?
- What terms & acronyms are too subject-specific?
- A talk about the same subject will be very different if you are talking to
  - Theoretical computer scientists
  - HPC engineers
  - Bioinformaticians
  - Evolutionary Biologists
- You will have to explain different things/concepts in more detail!

Slide layout

- Keep slides simple
- Use a **spell checker** for the slides
- Decide if you want to use American or British English
- Avoid numbering of type 10/50, 11/50 → audience will think: “... another 39 boring slides to go”
- Reduce text to the absolute minimum!
- Avoid busy slides including text & graphs & tables

  → if you need a complex slide use layers, i.e., first show text, then add graph, then add a table

  → direct the attention of your audience
- Avoid tables if possible → use intuitive graphical representations

Structure

- Provide an outline for your talk

  → re-use it at the beginning of each section

- Structure
  - State & Motivate the problem
    - Why is it interesting?
    - Why is it important?
  - Own contribution: very brief
    - What did you do/What did you contribute?
    - This is often very fuzzy, I have attended many talks where it was not clear for a long time what the contribution of the authors actually was
    - Throughout the talk, make it very clear:

      (i) what is prior knowledge

      (ii) what you did contribute

Structure

- Outline
- Intro & Motivation
- Own Contribution
- Abstract, but more detailed problem description

  → omit unnecessary details
- Describe your solution/contribution
- Experimental Results

  → experimental setup

  → HW & datasets used

  → results (if possible no tables, intuitive graphs)

  → comparison with competing approaches
- Conclusions & Future Work
- Acknowledgements: funding agencies, people who have helped you

Reporting Results

- e.g., parallel speedups

  → don't show execution time over processor plots

  → show speedups, much easier to interpret

- Showing graphs

  → label the *x* and *y* axis!

  → before discussing the graphs, say what the *x* and *y* represent!

  → don't show more than one graph per slide!

Acronyms

- I can't stand it when people use acronyms in texts without introducing them
- There are very few acronyms that are known to everybody
  - MPI is one of these …
  - But only at a HPC conference
- Don't use acronyms in slides
- People can not remember their meaning in such a short time

An example presentation

- Work on barriers
- Presented at IEEE Cluster in 2010
- I didn't have much time to prepare the slides
- By far not perfect
- I have commented the slides
  - Things I liked
  - Things I didn't like

Assessment of Barrier Implementations for Fine-Grain Parallel Regions on Current Multi-core Architectures

The title

The Authors
Who is giving the talk?

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Technical University of Munich

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Affiliation and
Contact details

Outline

- **Motivation**
- Type of parallel regions
- Barriers
- Test Applications
- Results
- Conclusions

Motivation

- Little is known about efficient barrier implementations on multi-cores using Pthreads and OpenMP
- Need for assessment on current multi-core architectures
- Focus on applications with large number of fine-grain parallel regions

  → applications where barrier performance is an issue
- Background: Bioinformatics application for reconstruction of evolutionary trees from DNA data

There's a bit too much text
On this slide + it's badly formatted

Questions

Sentence too long!

- Does barrier efficiency depend on
  - Specific multi-core architecture?
  - Memory and Cache utilization and access behavior of the application at hand?
- Best barrier implementation for Pthreads?
- Pthreads implementation required for non-expert users!

That's actually the motivation for Using Pthreads

Goals

Sentence maybe too long!
Not well-formatted

- Devise efficient barrier implementation
- Provide for barrier with deterministic reduction implementation
  - Reductions a + b + c + d must always be conducted in the same order, e.g.:
    - (a + b) + (c + d)
    - A reduction on the same numerical values must yield exactly the same result!
  - Not necessarily the case with OpenMP and MPI

Outline

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- **Type of parallel regions**
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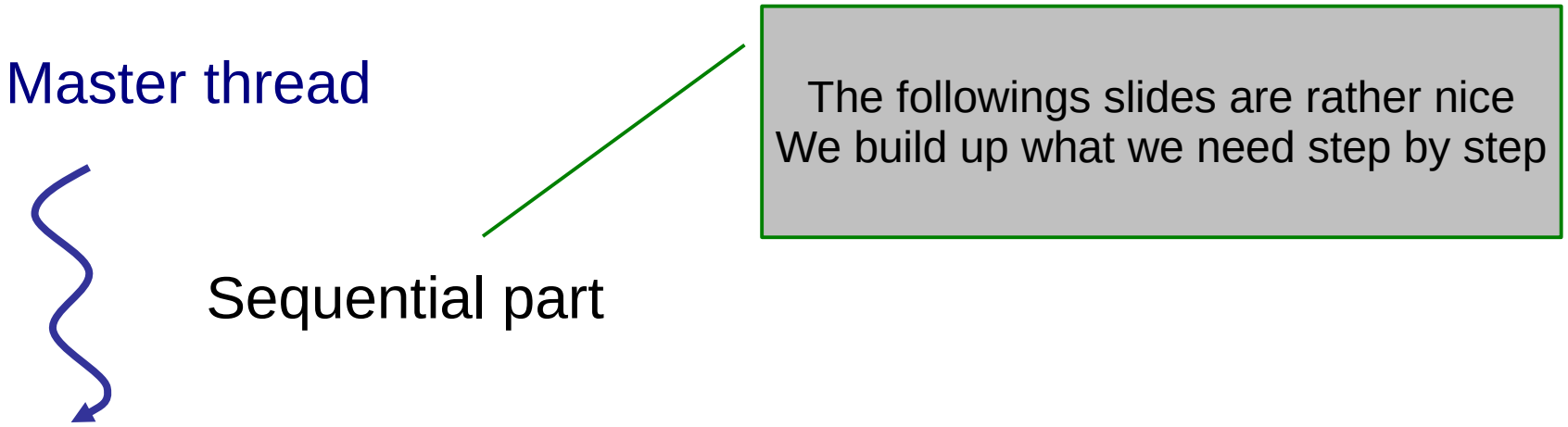
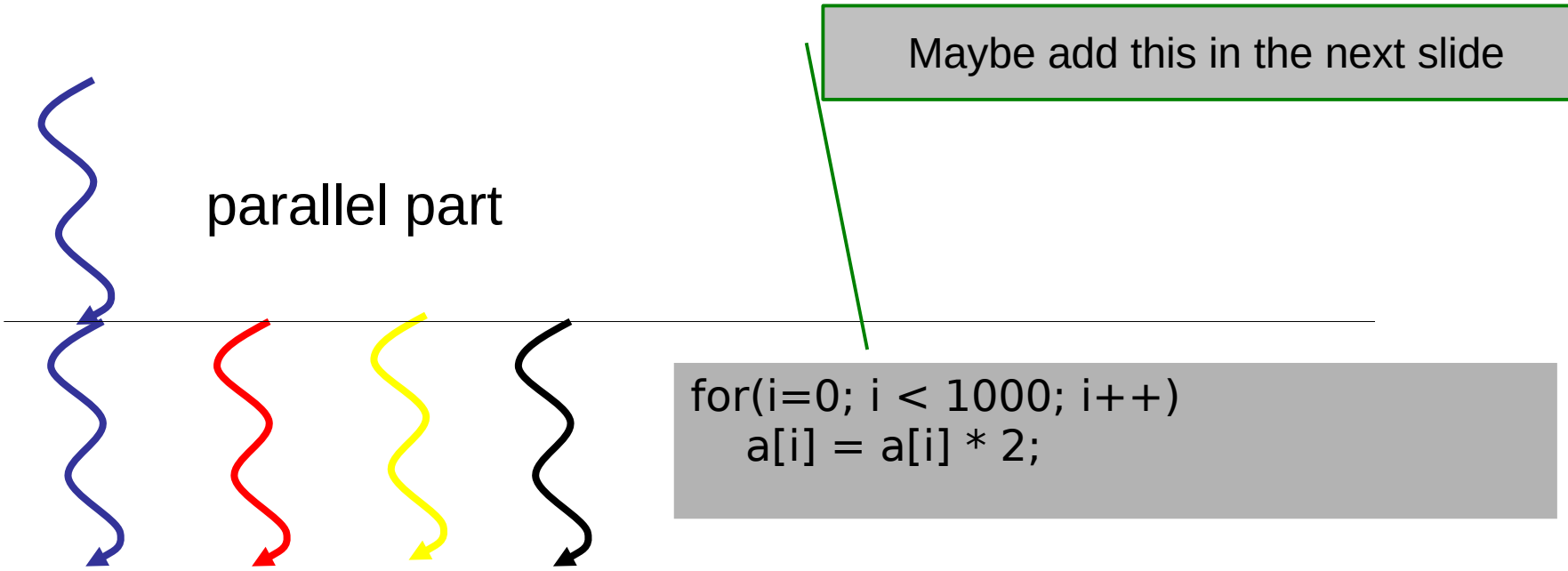
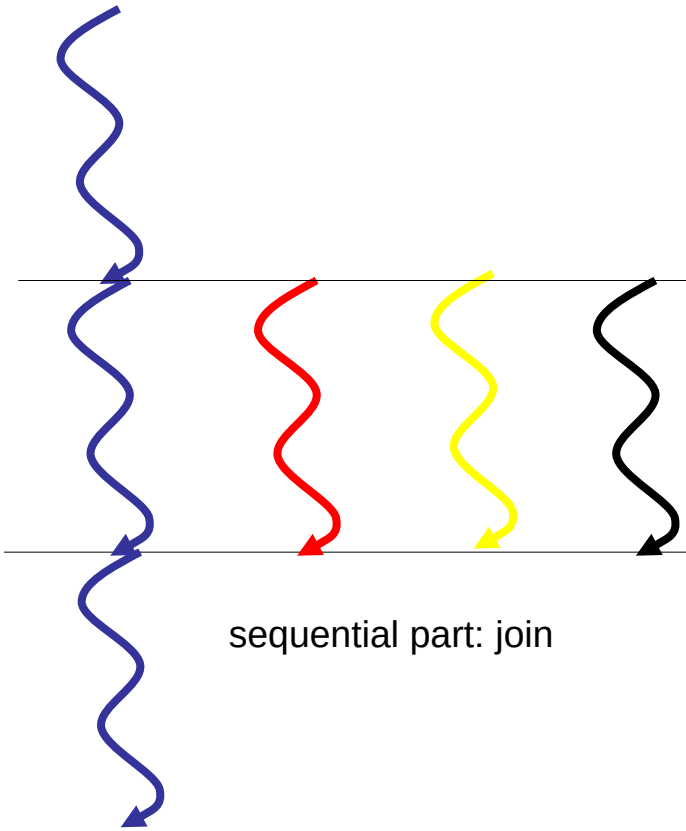
Thread Sync:
Fork-Join Model



Thread Sync: Fork-Join Model



Thread Sync: Fork-Join Model

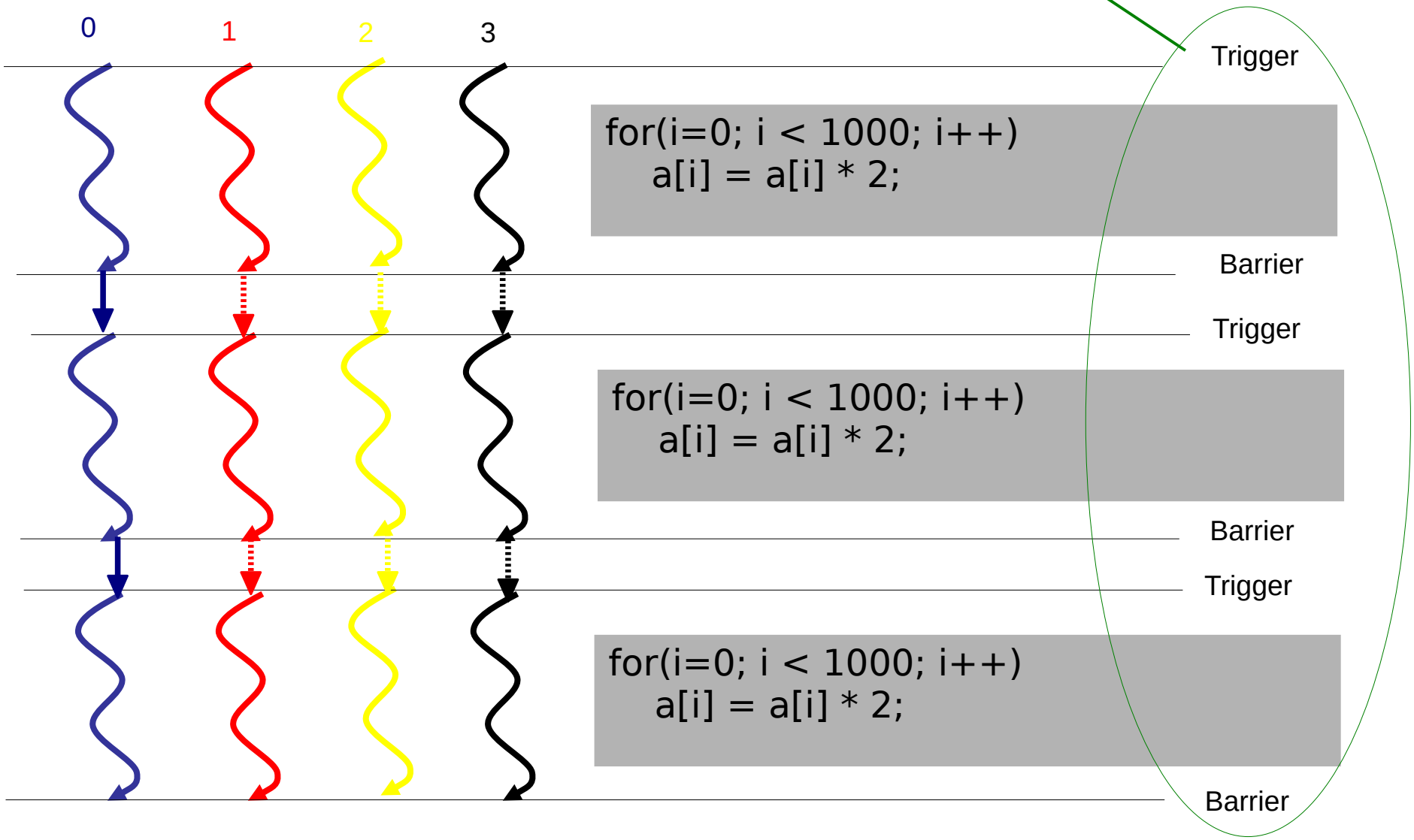


```
for(i=0; i < 1000; i++)
    a[i] = a[i] * 2;
```

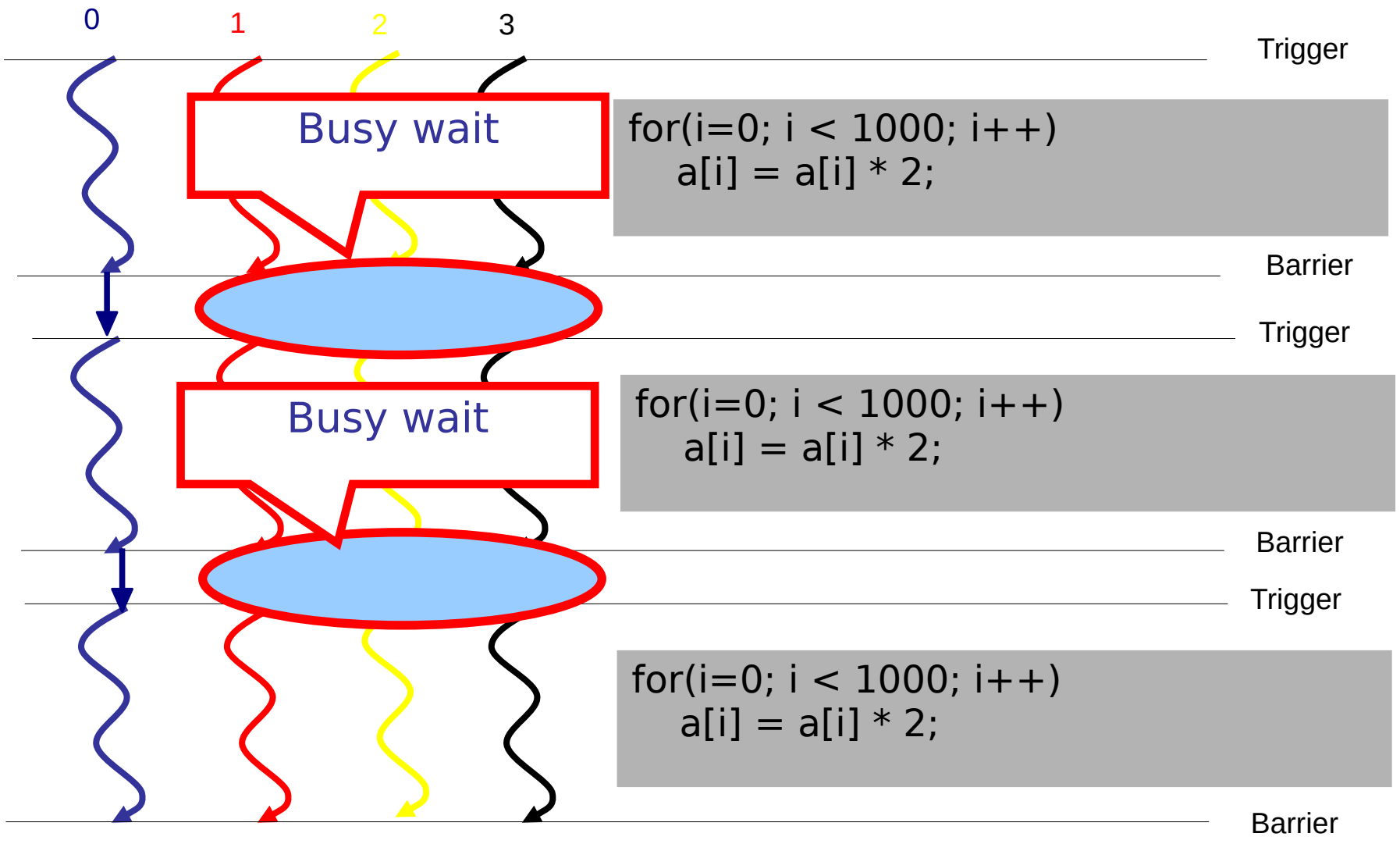
sequential part: join

Thread Sync: Barrier-based

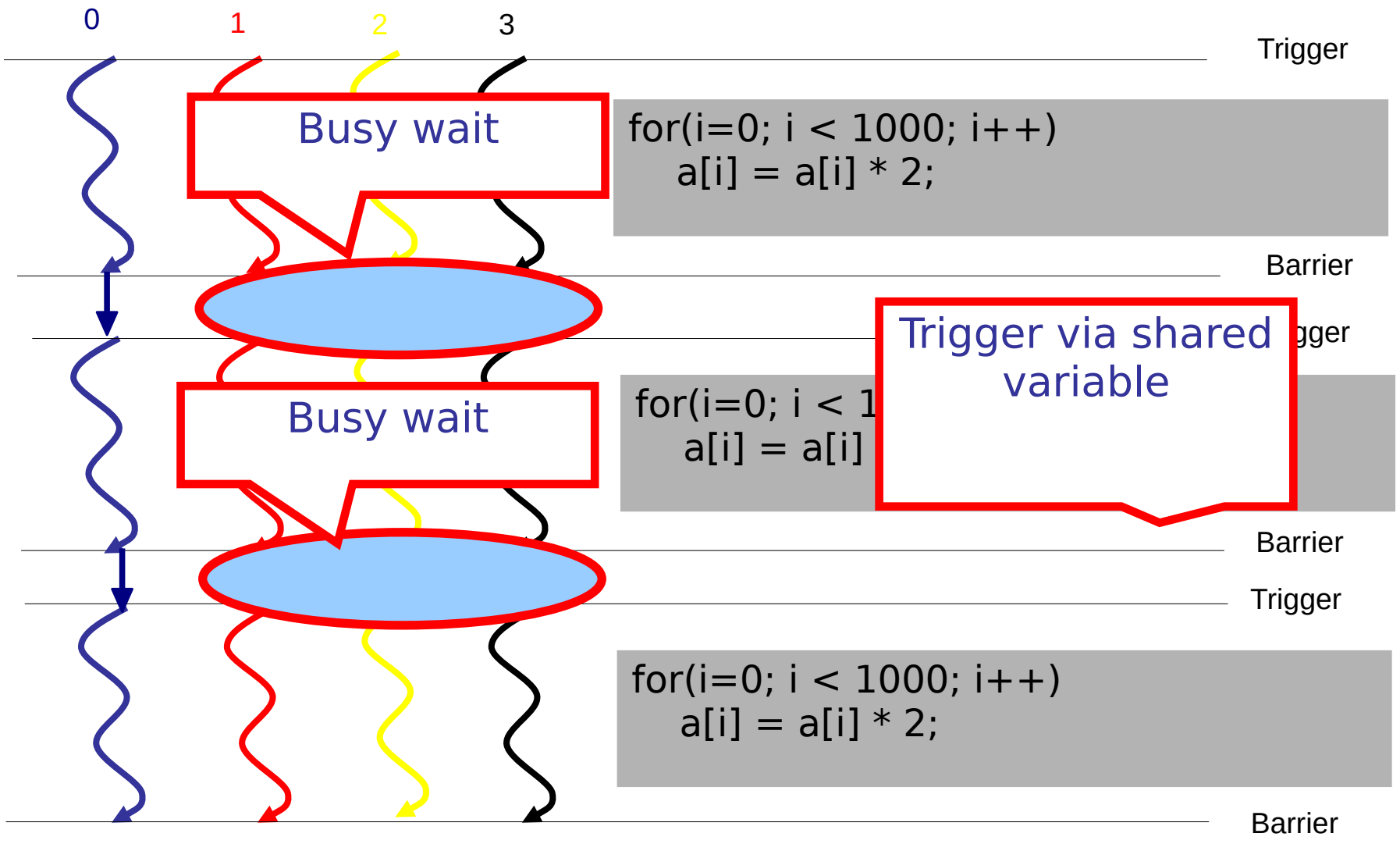
Should have added this on the next slide



Thread Sync: Barrier-based



Thread Sync: Barrier-based



Outline

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- **Barriers**
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Here I need to say that now I am Introducing the barriers we tested!

Master-Threads

Pasted in, badly formatted C code
Don't do this ;-)
Use pseudocode!

```
volatile int jobCycle = 0;

void masterBarrier(int tid, int n)
{
   jobCycle = !jobCycle;
   executeWork(tid, n);
   masterSync(tid, n);
}
```

Worker-Thread

```
void workerThread(int tid, int n)
{
   int mycycle = 0;
   while(1)
     {
        while(myCycle == jobCycle);
        myCycle = jobCycle;
        executeWork(tid, n);
        workerSync(tid, n);
     }
}
```

Lock-Free

```
void workerSync(int tid, int n)
{
   barrierBuffer[tid] = 1;
}

void masterSync(int tid, int n)
{
   int i, sum;
   do
      {
        for(i = 1, sum = 1; i < n; i++)
            sum += barrierBuffer[i];
      }
   while(sum < n);
}
```

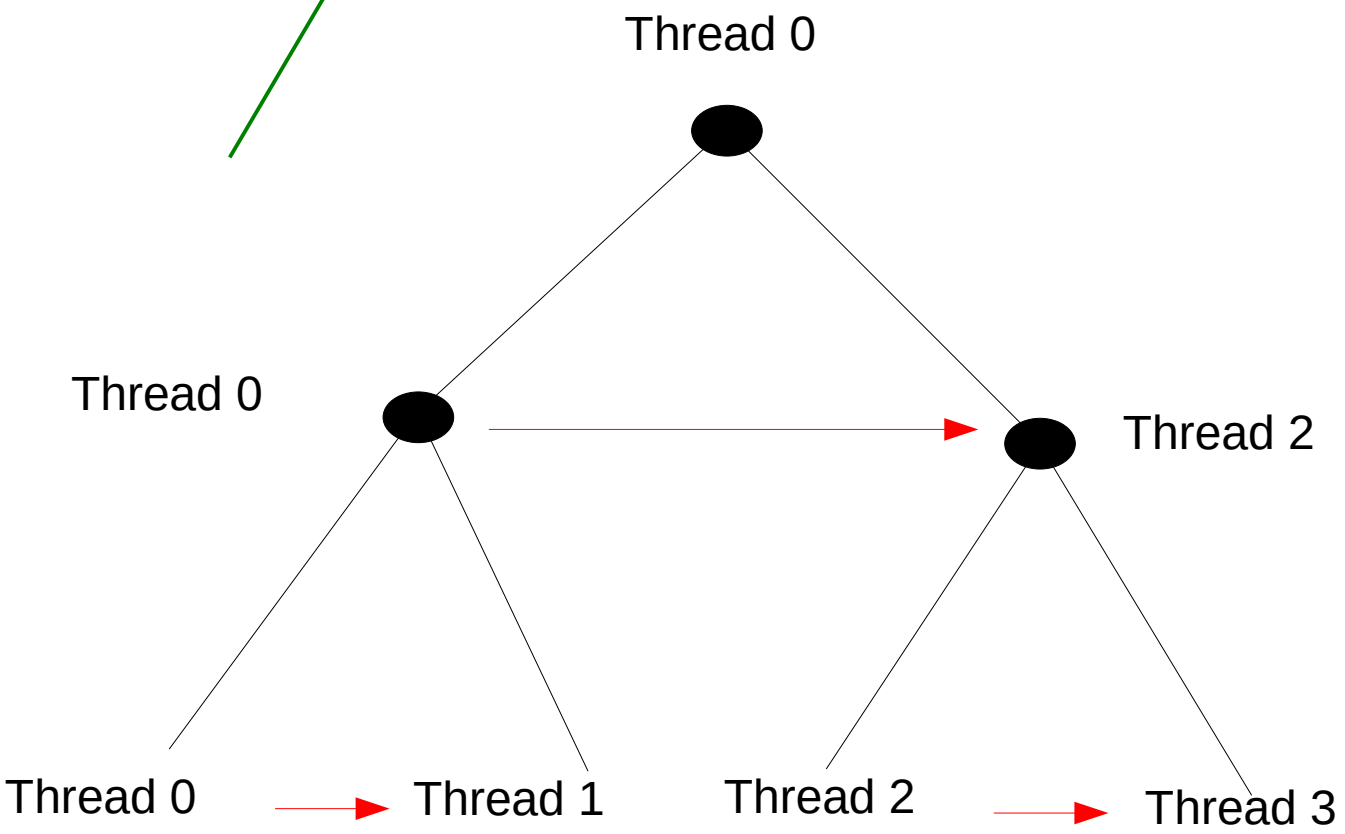
Lock-Free Padded

```
void workerSync(int tid, int n)
{
   barrierBuffer[tid * padding] = 1;
}

void masterSync(int tid, int n)
{
   int i, sum;
   do
      {
        for(i = 1, sum = 1; i < n; i++)
            sum += barrierBuffer[i * padding];
      }
   while(sum < n);
}
```

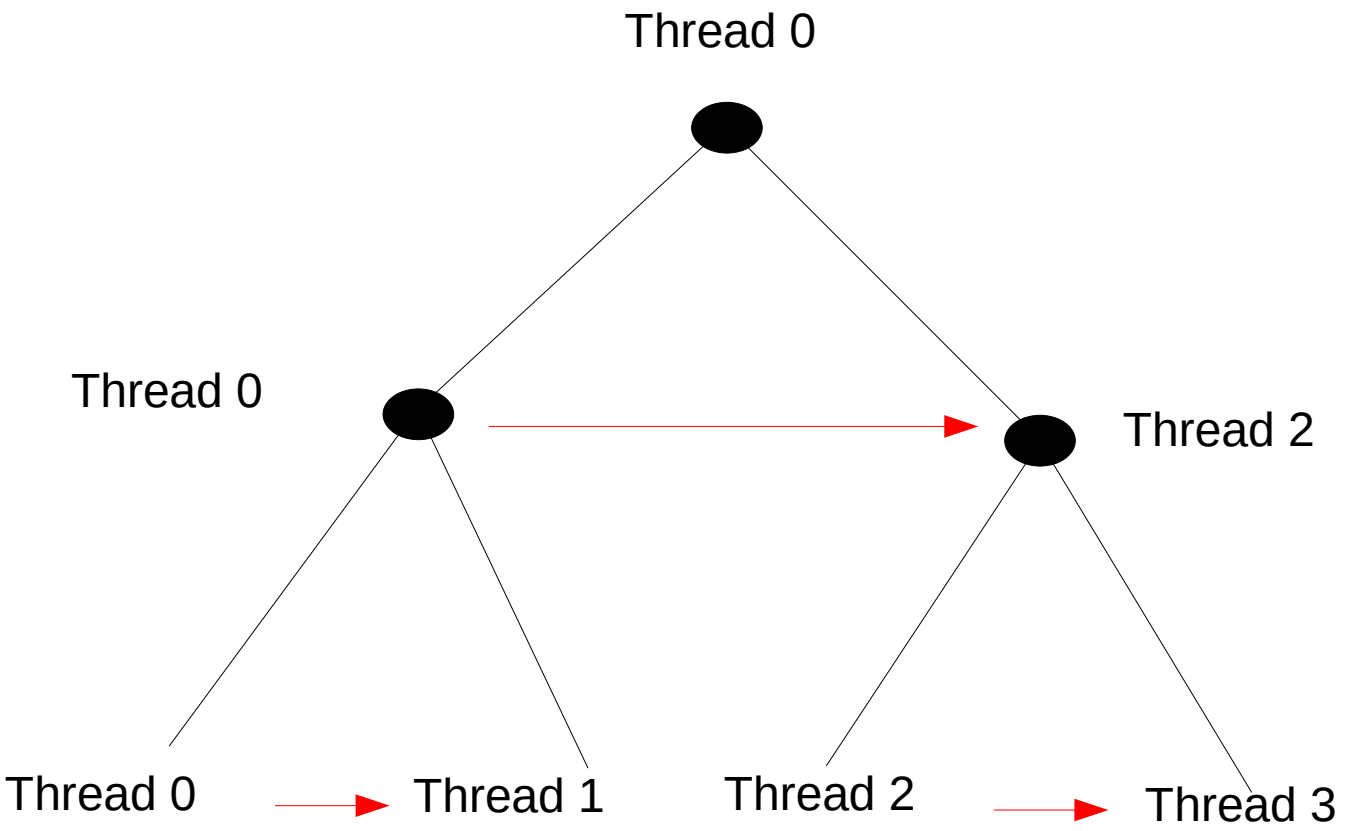
I should have provided an overview of the barrier implementations we Tested at the beginning of this part!

Recursive Lock-Free

That's a slide I like
One could have animated it though!



Recursive Lock-Free Padded



Intrinsic Atomic Increment

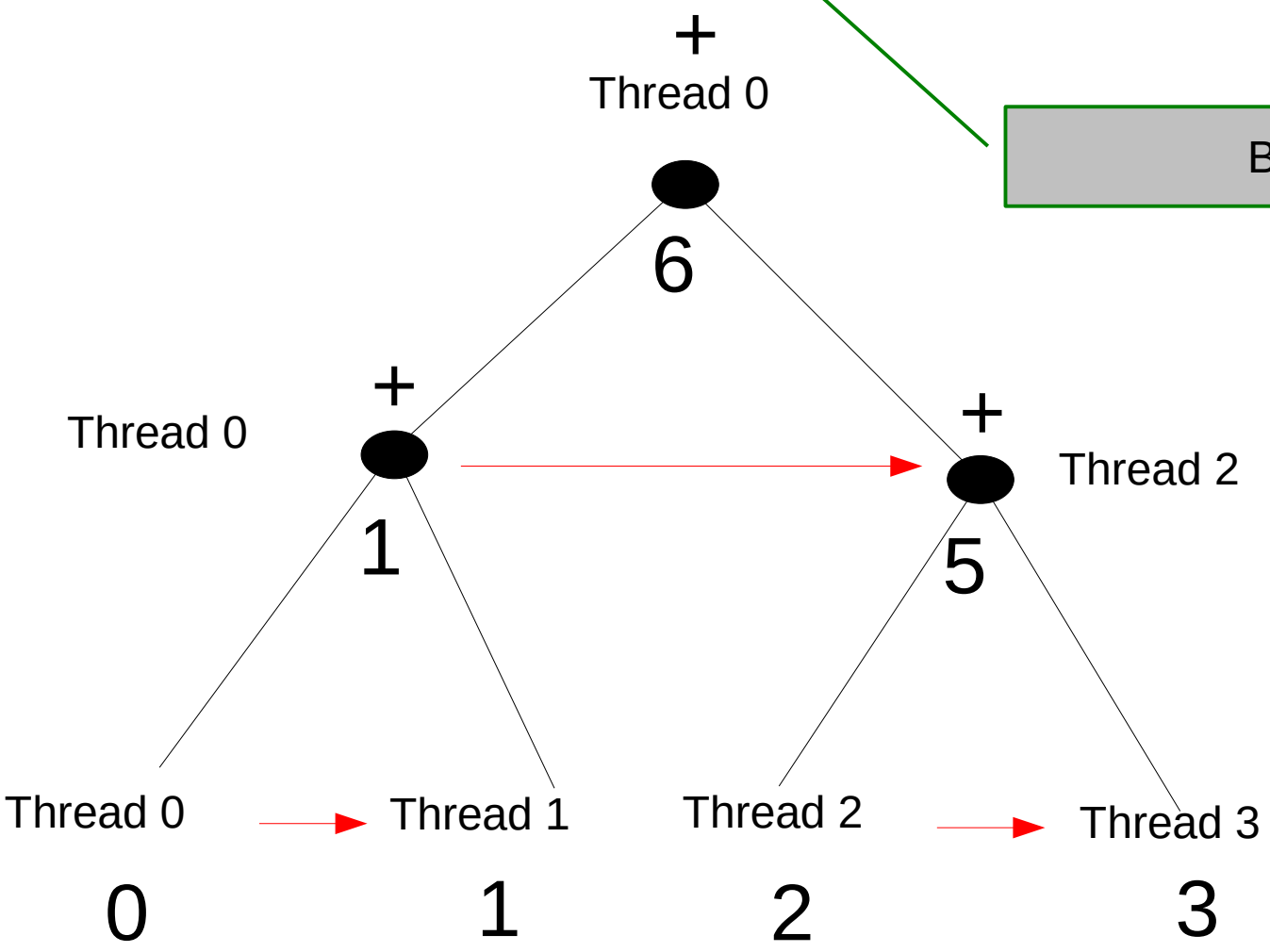
```
volatile int counter = 0;

void workerSync(int tid, int n)
{
	__sync_fetch_and_add(&counter, 1);
}

void masterSync(int tid, int n)
{
	int workers = n - 1;

	while(counter != workers);
	counter = 0;
}
```

Lock-Based

```
volatile int counter = 0;

void workerSync(int tid, int n)
{
	pthread_mutex_lock(&mutexCounter);
	counter++;
	pthread_mutex_unlock(&mutexCounter);
}

void masterSync(int tid, int n)
{
	int workers = n - 1;

	while(counter != workers);
	counter = 0;
}
```

Reduction Flavors

- Recursive “classic reduction”



Badly formatted!

Flat Reduction

- Threads store partial sums in shared array
- Master conducts reduction alone after barrier
- Tested with and without SSE3 vectorization
- Assumes that only one or two simple reductions are computed, e.g., reduction function is -,*,+

Too much text
I could have added a graphical representation here as well

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Test Applications

- Synthetic Benchmarks
  - Without workload
  - With workload
- Real Benchmark
  - RAxML Bioinformatics application

I don't say what I mean by workload here!

Synthetic Benchmarks

Badly formatted!

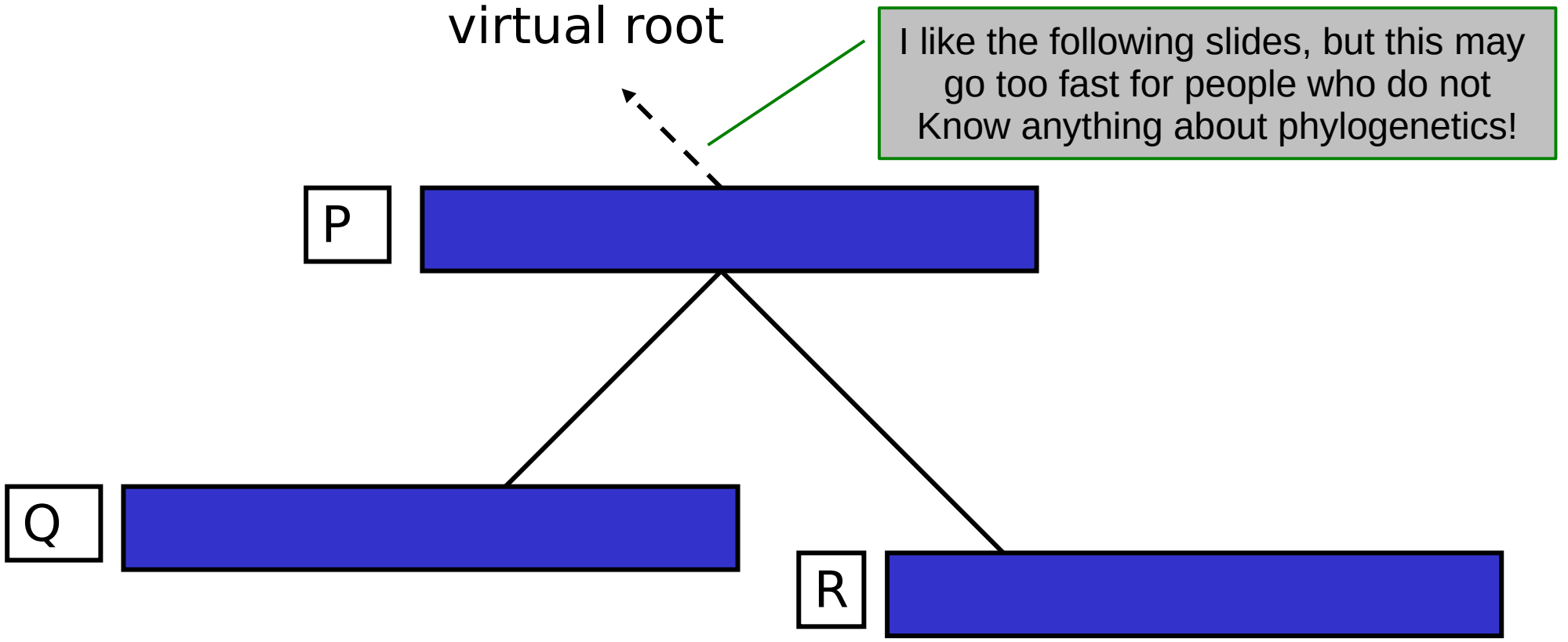
- With workload
  - 3 arrays v1, v2, v3 of length *M*
  - compute “v3[i] = v1[i] * v2[i]” *N* times with intermittent barriers
- Without workload
  - Set *M* to zero :-)
- Variables *N* and *M* are set at compile time
- Use of mmap() to control array allocation
- Cache utilization controlled by *M*

Real Workload

- Pthreads parallelization of RAxML
- RAxML: widely used tool for inference of evolutionary trees from DNA data
- Fine-grain production-level Pthreads parallelization
- Floating-point and memory intensive
- Considered subset of the phylogenetic likelihood function:
  - requires largest amount of sync
  - Two reductions on 1st and 2nd derivative of the likelihood (Newton-Raphson procedure)

Too much & partially unnecessary text

Loop Level Parallelism

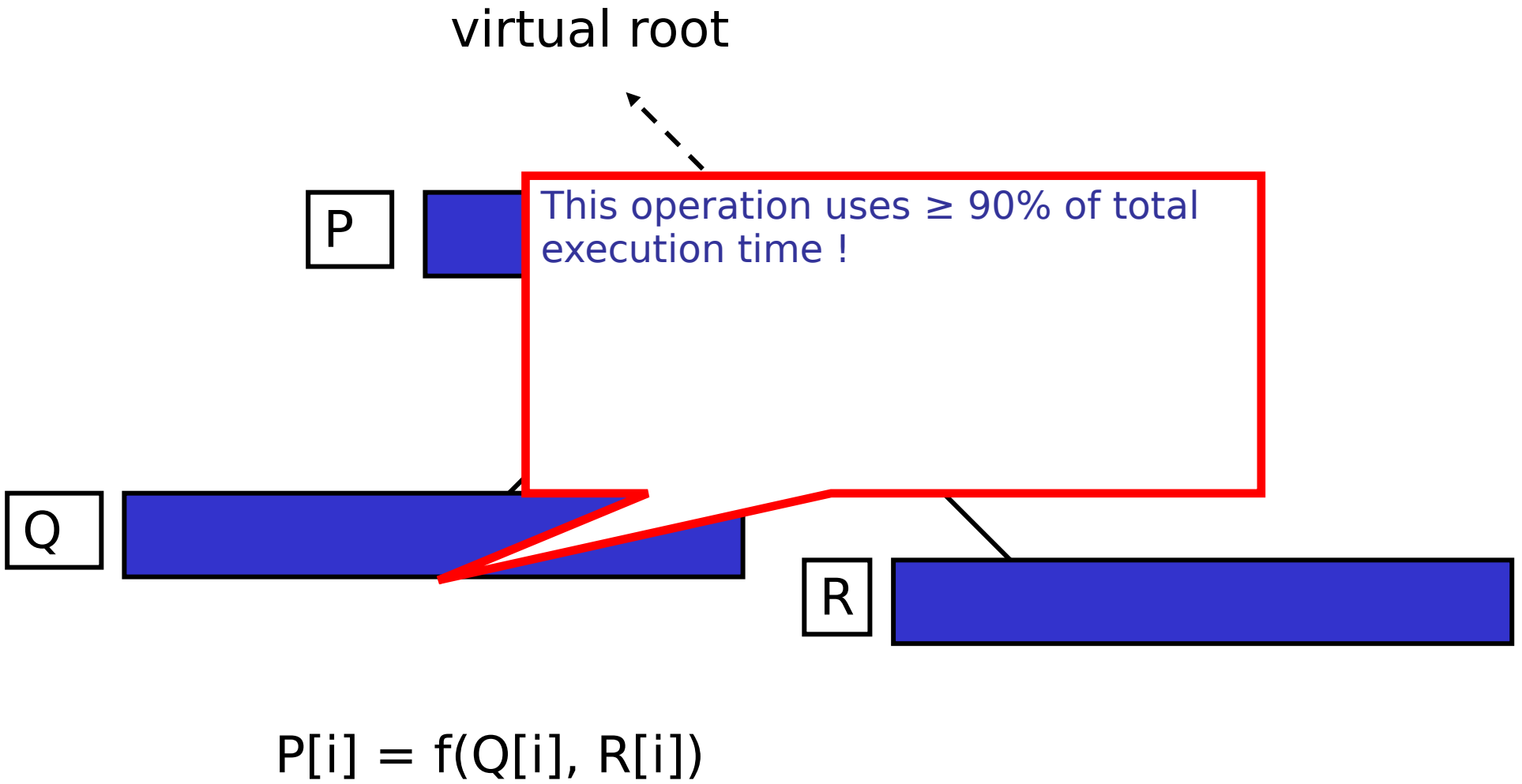


I like the following slides, but this may go too fast for people who do not Know anything about phylogenetics!

P[i] = f(Q[i], R[i])

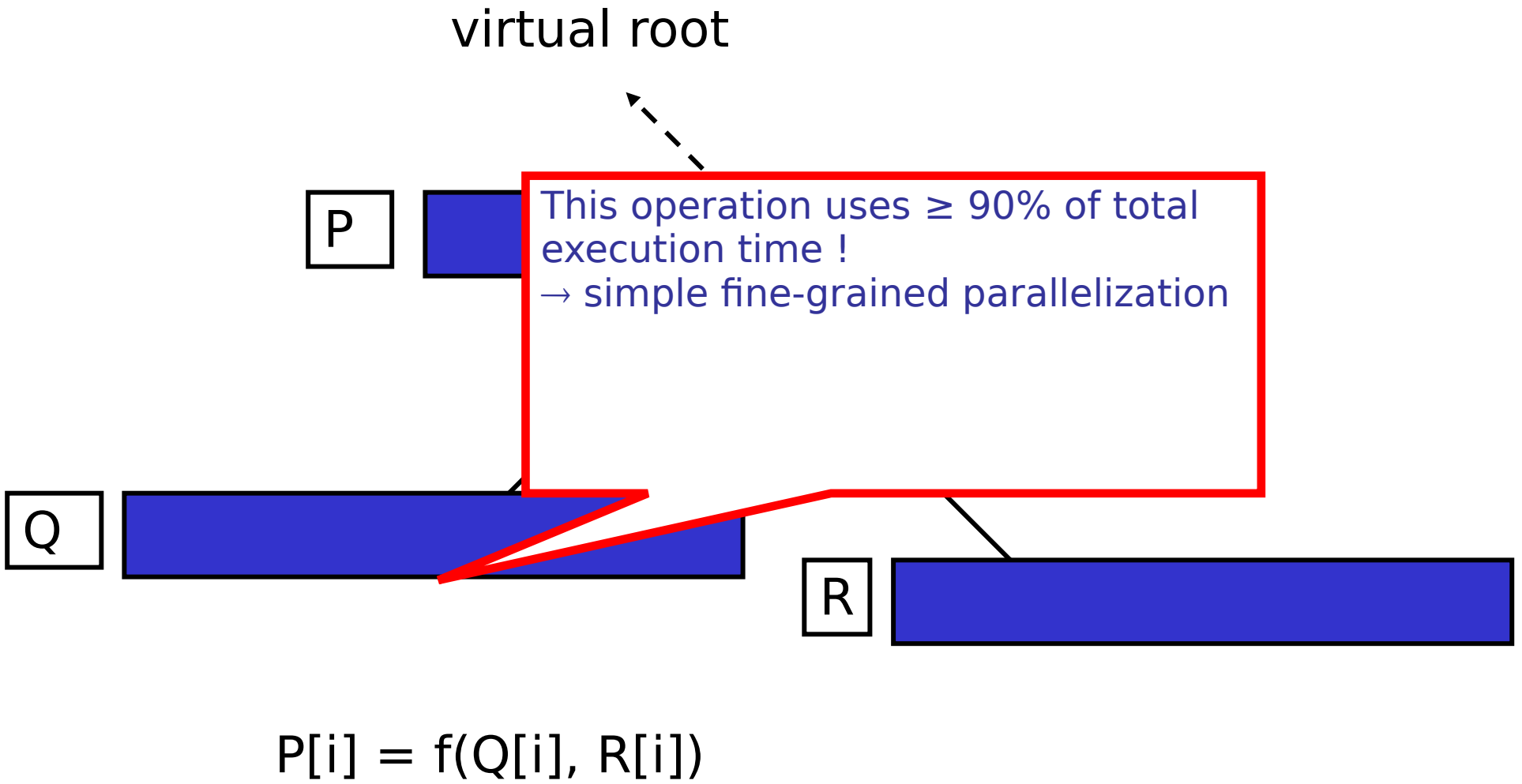
This should pop up on a second slide

Loop Level Parallelism



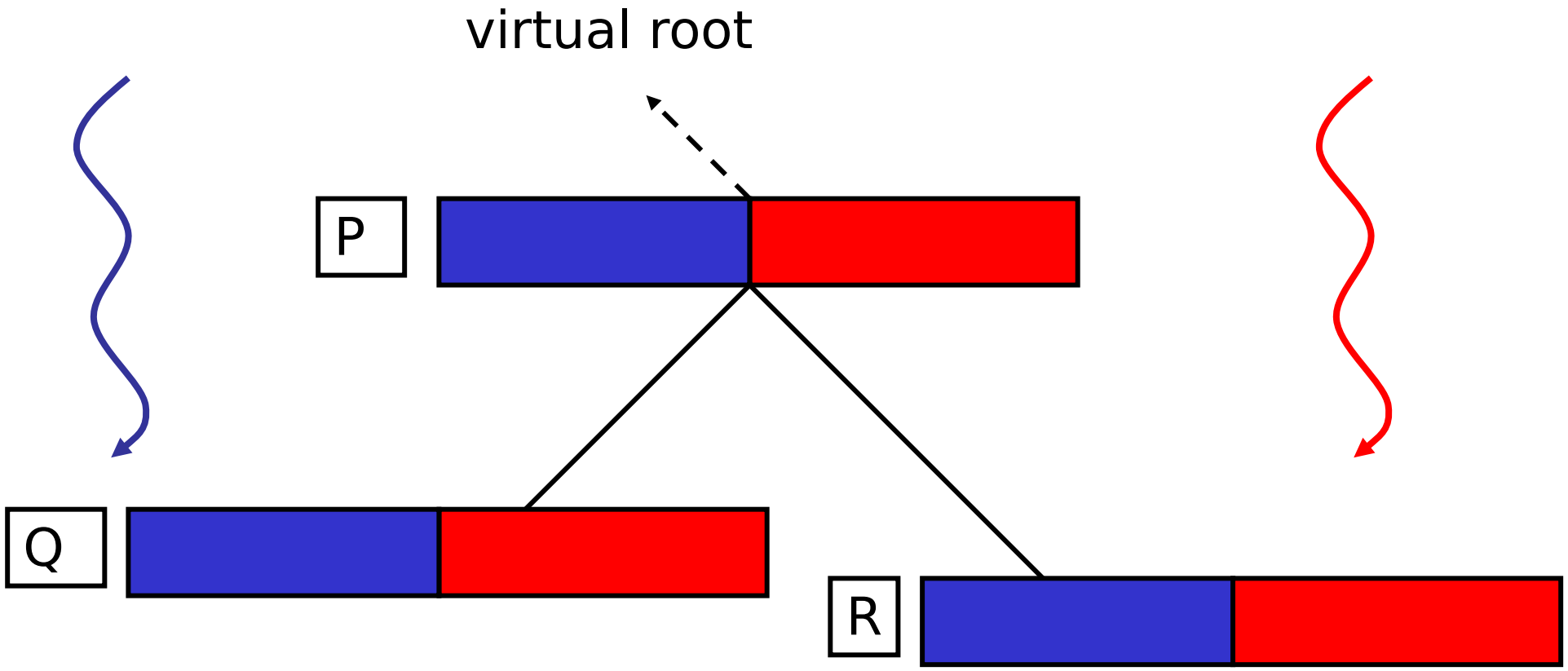
P[i] = f(Q[i], R[i])

Loop Level Parallelism

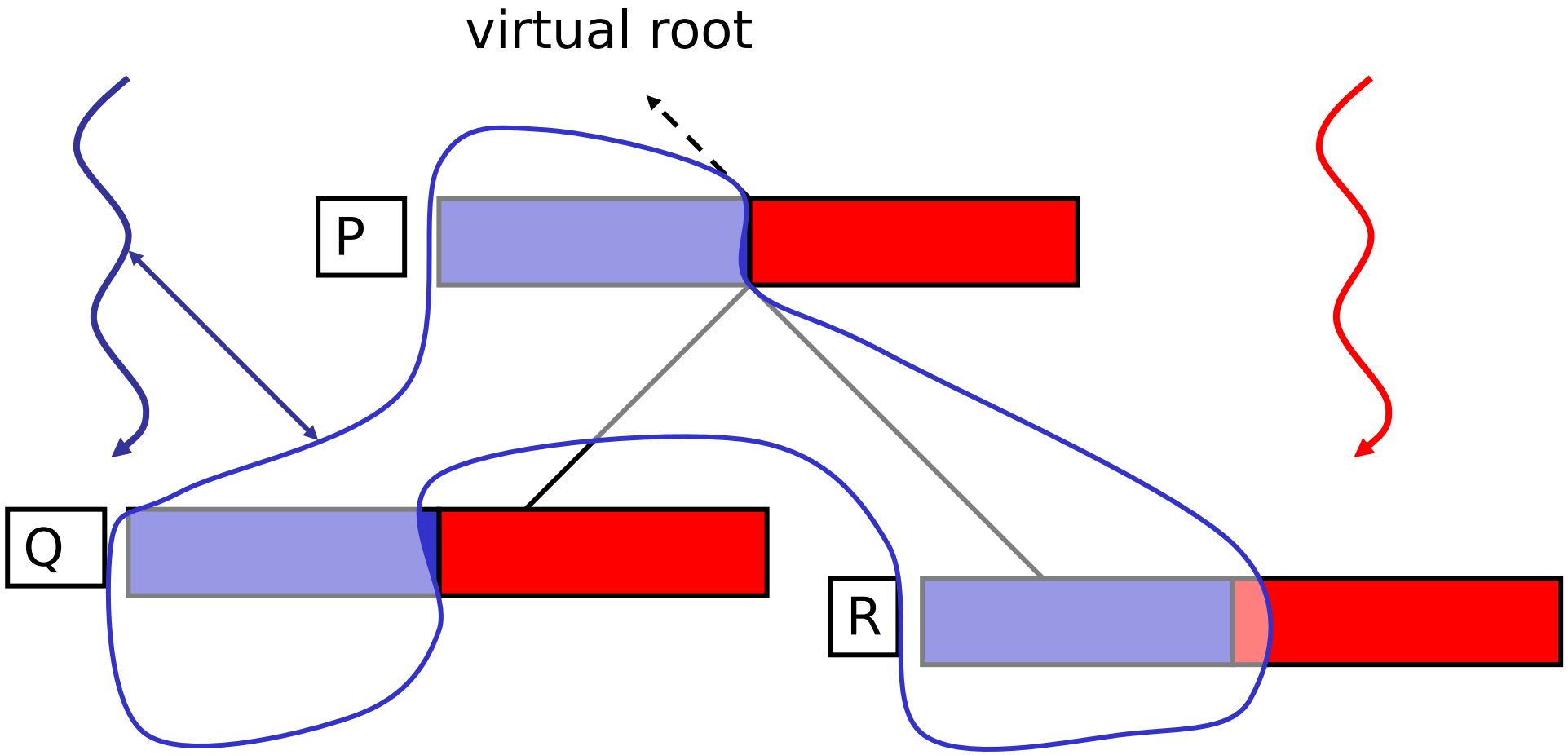


P[i] = f(Q[i], R[i])

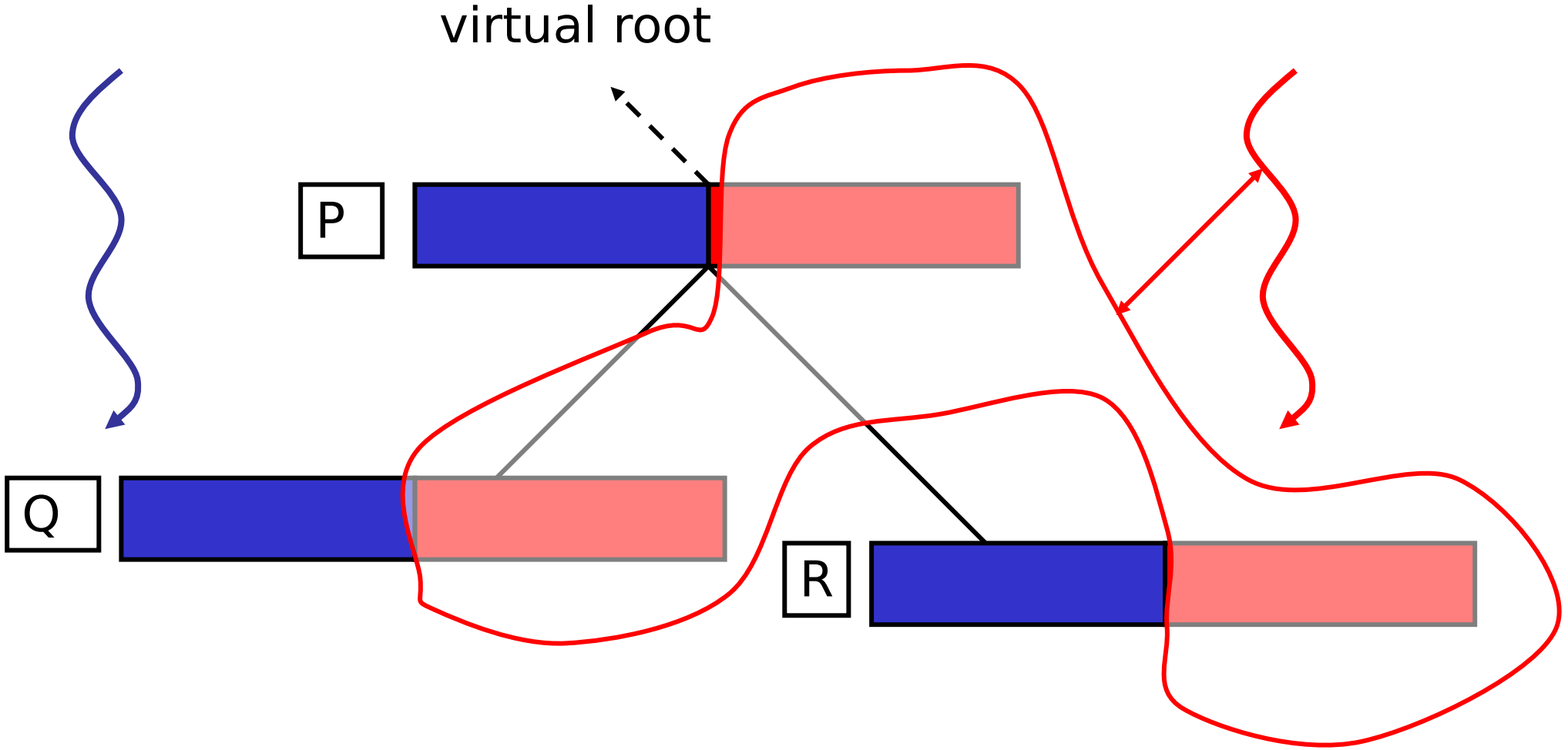
Loop Level Parallelism



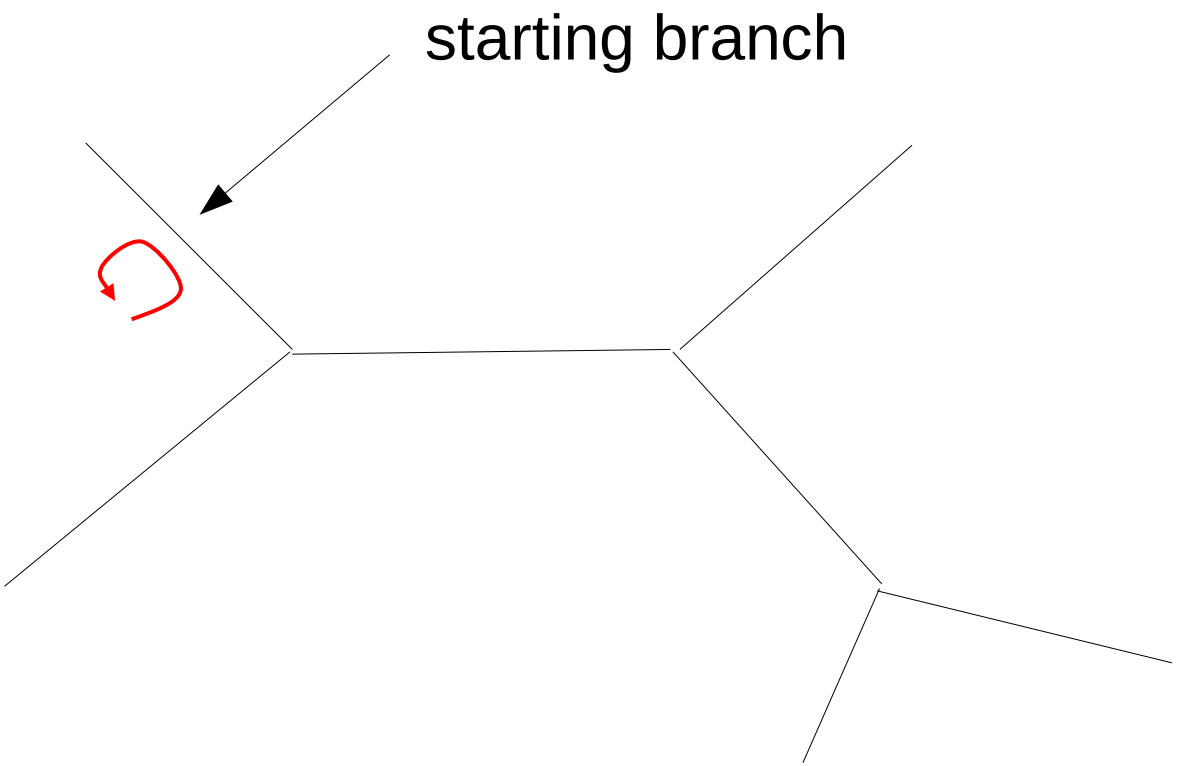
Loop Level Parallelism



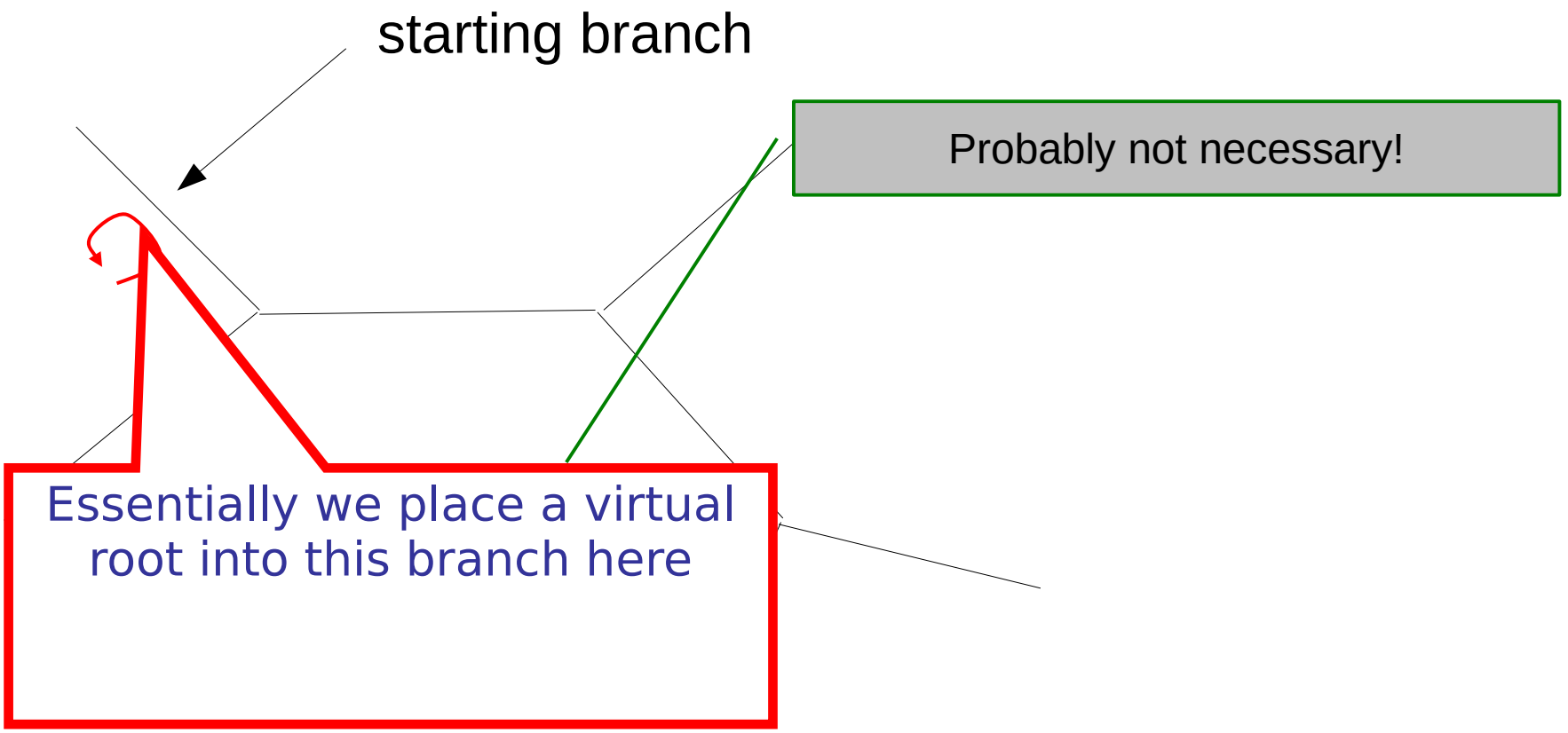
Loop Level Parallelism



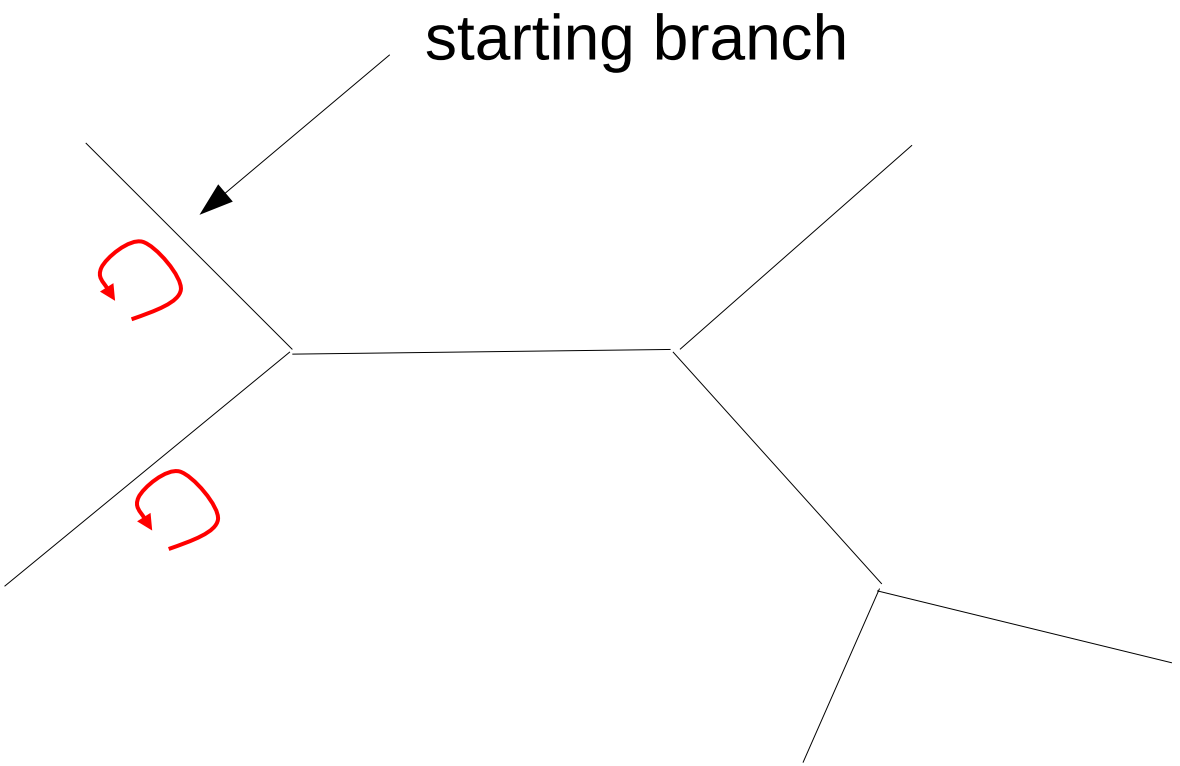
Branch Length Optimization



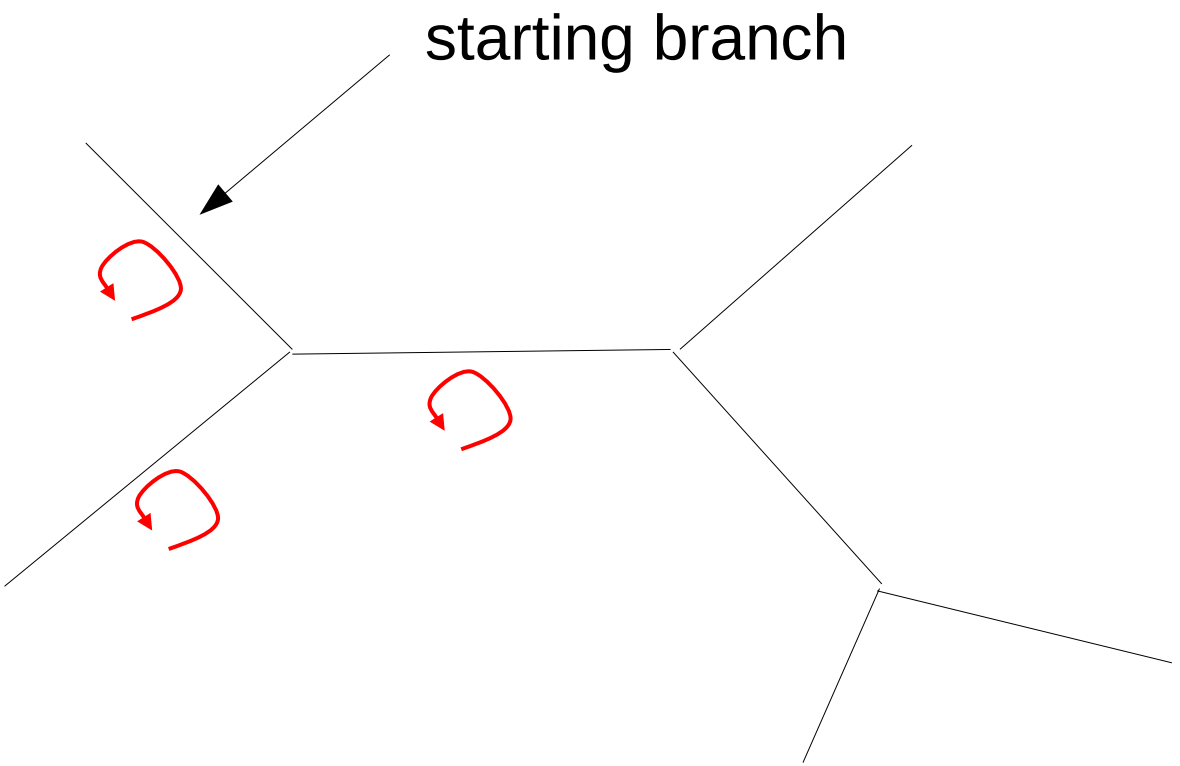
Branch Length Optimization



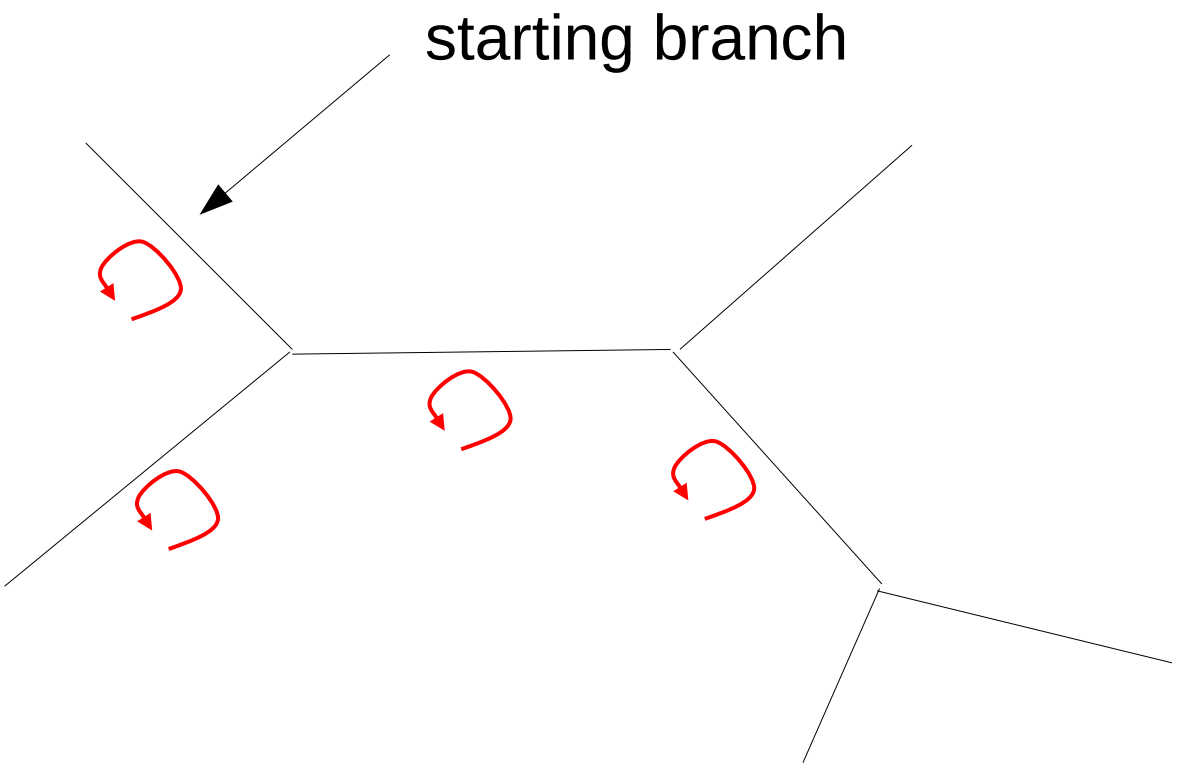
Branch Length Optimization



Branch Length Optimization



Branch Length Optimization



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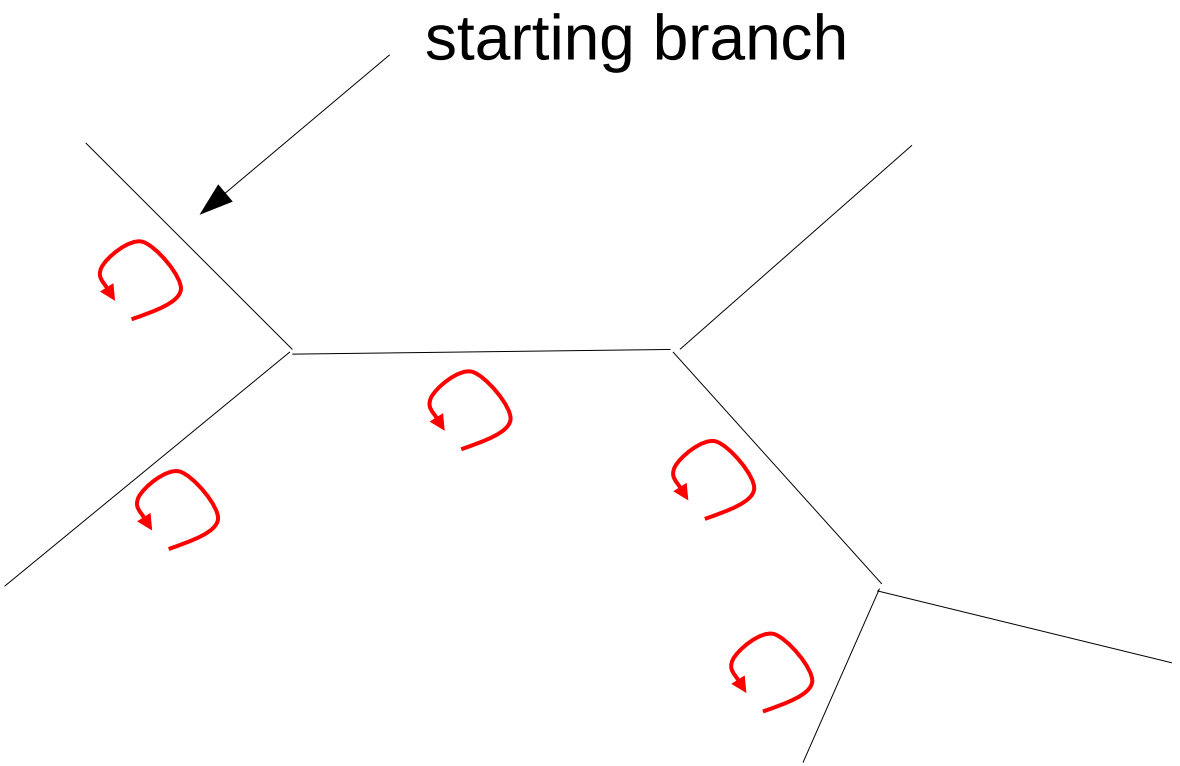
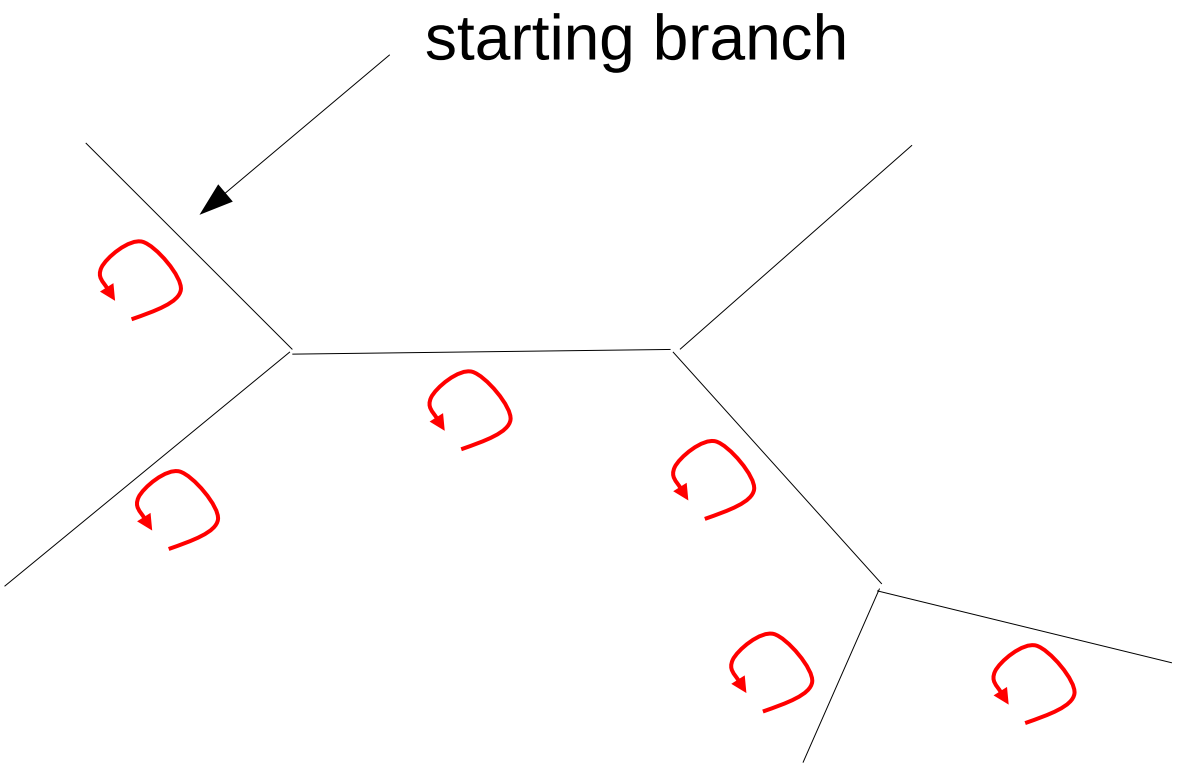
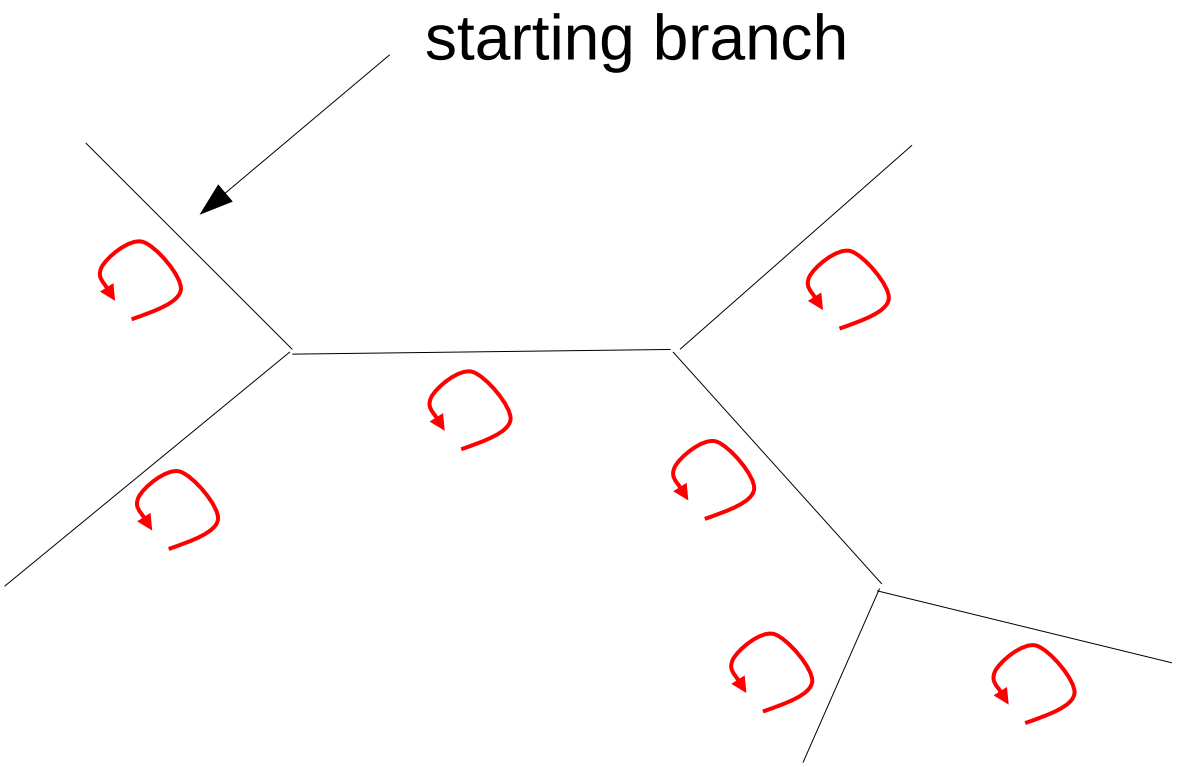


Branch Length Optimization



Branch Length Optimization



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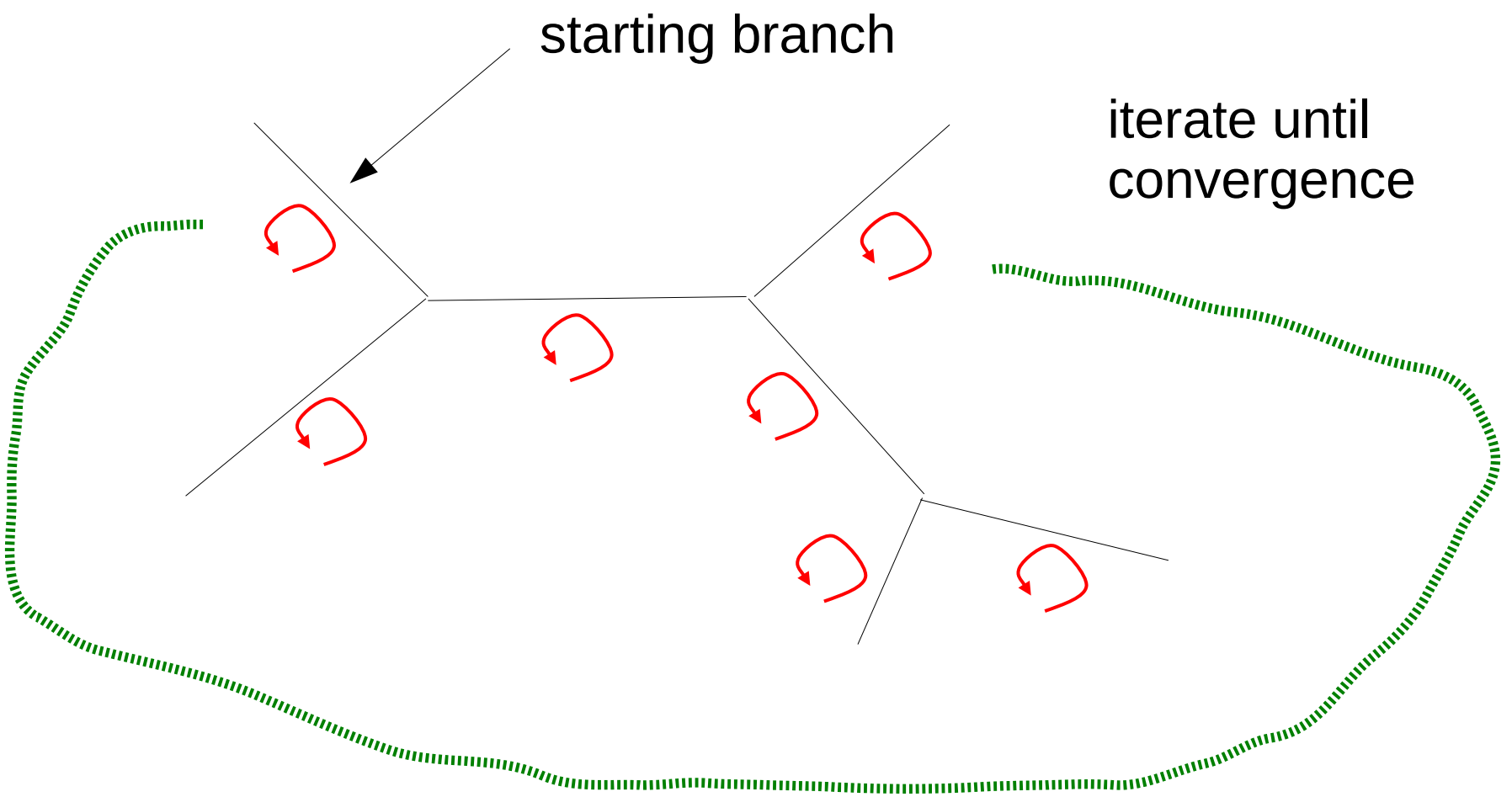
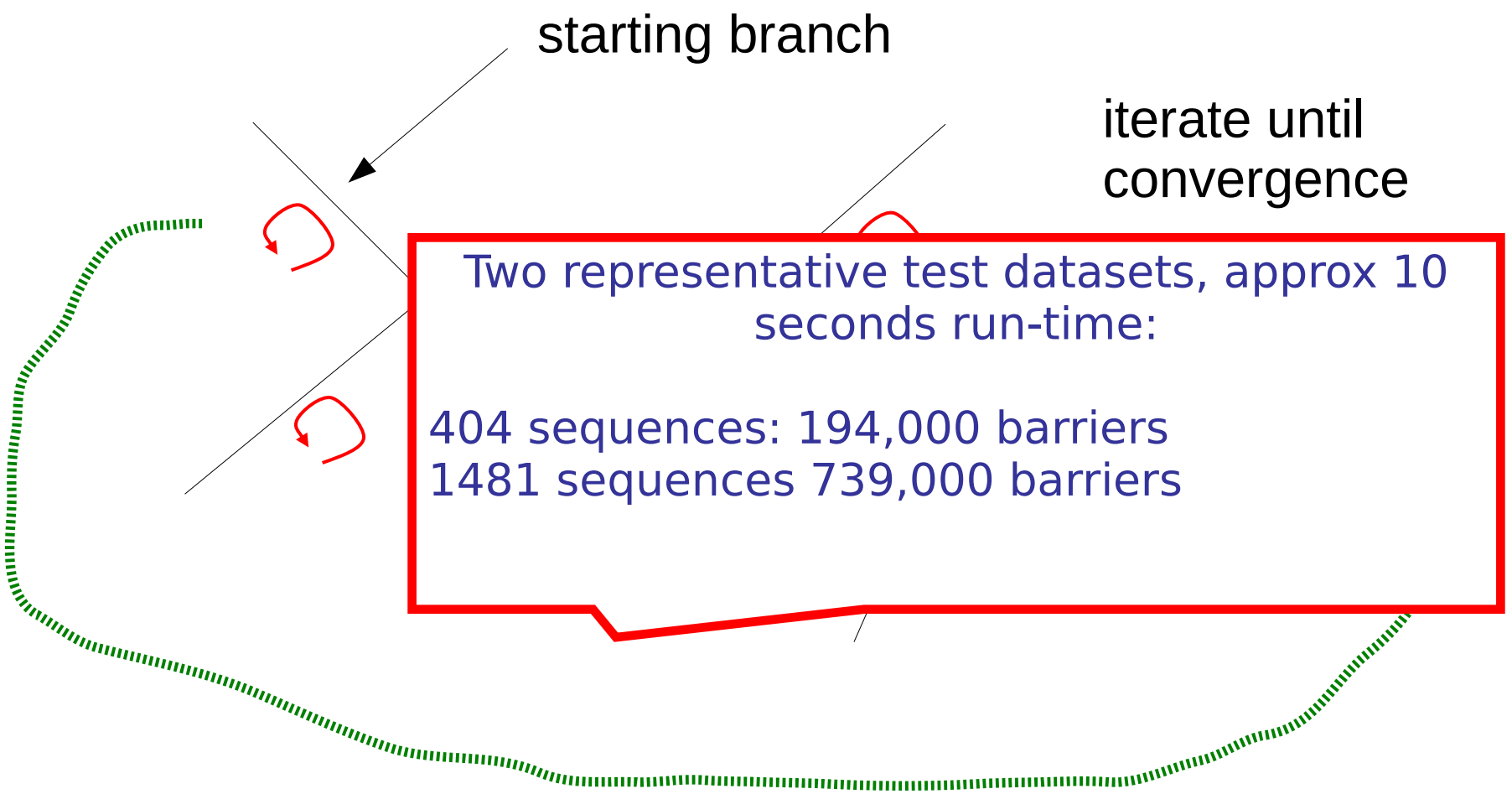


Branch Length Optimization



Outline

- Motivation
- Type of parallel regions
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- **Results**
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Test Platforms

- 2-core Intel Core2 Duo
- 4-core Intel Core 2 Quad
- 4-core Intel Core i5
- 8-core Intel Nehalem
- 16-core AMD Barcelona
- 32-core AMD Sun x4600
- 24-core AMD Sun x4440

The list looks ugly! We need the details here.
I should have sub-divided it
into Intel and AMD systems!

Synthetic without workload

This is something you should never do ;-)
→ represent numerical results graphically!

Table I
EXECUTION TIMES (SECONDS) FOR THE SYNTHETIC BENCHMARK WITHOUT WORKLOAD ($N := 10,000,000, M := 0$).

System	core2d (2T)	core2q (4T)	core i5 (4T)	Nehalem (8T)	Barcelona (16T)	x4440 (24T)	x4600 (32T)
Lock-Free	**2.366**	7.315	4.887	15.589	50.084	66.97	111.991
Lock-Free-Padded	2.370	**6.577**	4.788	**13.559**	**47.819**	**63.488**	**104.804**
Recursive	2.390	8.337	5.200	17.258	70.774	112.151	180.155
Recursive-Padded	2.396	7.554	5.460	14.883	51.462	73.222	121.957
Atomic-Inc-Add	2.432	7.439	**4.640**	14.682	48.799	65.590	107.950
Mutex-Inc-Add	3.121	60.92	20.236	105.135	438.651	636.085	1413.045

Synthetic with workload

This is something you shouldn't do ;-)

Table II
EXECUTION TIMES (SECONDS) FOR THE SYNTHETIC BENCHMARK WITH WORKLOAD ($N := 100,000, M := 10,000$).

System	core2d (2T)	core2q (4T)	core i5 (4T)	Nehalem (8T)	Barcelona (16T)	x4440 (24T)	x4600 (32T)
Lock-Free	9.087	7.753	8.675	8.343	14.305	16.738	12.291
Lock-Free-Padded	9.093	7.717	8.676	**8.328**	14.324	**15.466**	12.343
Recursive	9.086	7.762	8.679	8.368	14.469	17.223	12.963
Recursive-Padded	9.105	**7.700**	8.681	8.350	14.344	15.978	12.470
Atomic-Inc-Add	**9.058**	7.747	**8.672**	8.365	**14.268**	15.996	**12.269**
Mutex-Inc-Add	9.025	7.997	8.794	9.053	18.097	17.204	23.507

RAxML 404 sequences

Table III

EXECUTION TIMES (SECONDS) FOR PARALLEL BRANCH LENGTH OPTIMIZATION WITH RAXML ON A DATASET WITH 404 ORGANISMS USING ALTERNATIVE BARRIER IMPLEMENTATIONS ON THE X4600, BARCELONA, NEHALEM, AND X4440 SYSTEMS.

System	x4600 (32)	Barcelona (16)	Nehalem (8)	x4440 (24)
Lock-Free	9.260	16.421	22.916	12.559
Lock-Free-SSE3	**9.234**	**16.378**	**22.885**	**12.533**
Lock-Free-Padded	9.267	16.433	22.969	12.630
Recursive	10.444	16.679	22.919	13.058
Recursive-Padded	9.387	16.504	23.016	12.656
Recursive-Padded-Red	9.407	16.510	22.934	12.725
Atomic-Inc-Add	11.669	17.073	22.916	12.583
Mutex-Inc-Add	37.503	22.303	23.298	20.254

RAxML 1481 Sequences

Table IV
EXECUTION TIMES (SECONDS) FOR PARALLEL BRANCH LENGTH OPTIMIZATION WITH RAXML ON A DATASET WITH 1,481 ORGANISMS USING ALTERNATIVE BARRIER IMPLEMENTATIONS ON THE X4600, BARCELONA, AND NEHALEM SYSTEMS.

System	x4600 (32)	Barcelona (16)	Nehalem (8)
Lock-Free	11.678	13.803	15.000
Lock-Free-SSE3	11.565	**13.705**	14.982
Lock-Free-Padded	11.590	13.734	14.920
Lock-Free-Padded-SSE3	**11.486**	13.722	14.896
Recursive	16.743	15.141	15.090
Recursive-Padded	11.935	13.946	14.996
Recursive-Padded-Red	12.062	13.936	**14.890**
Atomic-Inc-Add	21.039	16.624	15.171
Mutex-Inc-Add	126.252	39.994	18.908

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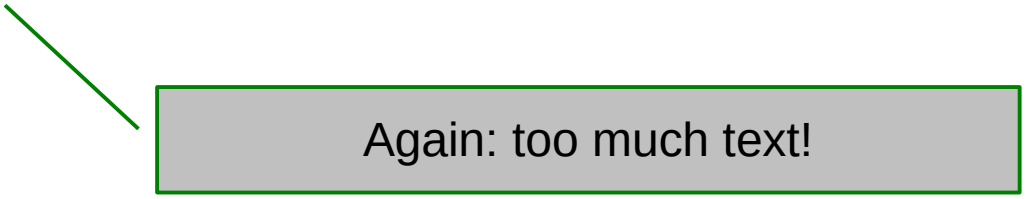
Conclusions

- Intrinsic atomic increment does not yield optimal performance
- Performance of different barrier flavors depends on cache utilization of application
- Lock-free barriers and SSE3-based flat reductions appear to work best across all platforms



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Nick Pattengale, Sandia

Michael Ott, TUM

Andre Aberer,
TUM

Fernando Izquierdo,
TUM

Christian v. Mering & Manuel Stark
University of Zürich

Wayne Pfeiffer, SDSC

Thank you for your Attention !

Zakros, Crete, Greece, September 2008

Summary

- This was an “okay” presentation, but
- Too much text
- Sometimes lacking a clearer structure!
- Could have included more pictures
- Result section
  - → copied & pasted tables from paper
  - → don't do this

Today

- How to give a scientific presentation
- **How to write a technical report/scientific paper**

General structure

- Meaningful (catchy?) Title, catchy title, for instance:

  “Short tree, long tree, right tree, wrong tree: new acquisition bias corrections for inferring SNP phylogenies”
- Authors and affiliations
- Abstract
  - Motivation
  - Problem Statement
  - Own Contribution
  - Results
- Introduction and Motivation

General structure

- Related work (can also be moved further to the end)
- Own contribution, e.g.,
  - Algorithm
  - Parallelization
  - Model
- Results
  - Experimental setup
    - How were test datasets generated?
    - What kind of HW was used?
    - How can the experiments be reproduced?
      - → reproducible science
      - → make SW and datasets available for download!
      - → Archive the data for 10 years!
      - → Archive data when the paper is accepted for publication!

General structure

- Results
  - Experimental Setup
    - Datasets used
    - HW platforms used
    - Compilers used
  - Results
    - Graphs, speedup plots, tables
    - Comparison to competing SW, algorithms etc
- Conclusion and Future Work
- Acknowledgements
  - Funding agencies
  - Colleagues who helped

Biology Papers

- The structure is a bit different
- Abstract
- Introduction
- Materials & Methods (e.g., field work, sequencing, bioinformatics analysis, etc.)
- Results
- Discussion ← this is longer and more important than in CS, because results are typically more fuzzy
- Acknowledgements

Writing papers

- Be exact & precise
- Be exact & precise
- Be exact & precise
- Omit unnecessary information
- Don't be wordy, be concise
- Use **short sentences**!
- Avoid colloquial expressions!
- Avoid qualitative words: much, little, good, few
- Quantify things!
- Don't say “in most cases our code performed well” → “in 65% of the cases our code showed an accuracy improvement exceeding 5% over ...”

Writing papers

- In engineering-style papers
- Always provide a rationale for design choices!

  Instead of “We use an array representation with binary search for storing and retrieving elements.” → “We use an array representation with binary search for storing and retrieving elements, because binary search trees performed worse for the problem at hand.”
- In English: Sentences are generally much shorter
- Don't show that you are educated (as sometimes done in German) by writing long sentences using elaborate vocabulary
- **Keep Things Simple!**

Writing papers

- If your English is generally mediocre don't build in “100 Dollar words” you looked up in the dictionary → this just sounds ridiculous
- Occasional language jokes are allowed, e.g., using phrases such as “Based on the prolegomena”
- Use a spell checker
- Use a spell checker
- Use a spell checker

Writing papers

- In Latex add a ~ after . in the middle of a phrase
- Properly introduce acronyms
- Say what acronyms mean the first time you use them
- Use/introduce acronyms consistently to make the text shorter
- E.g., multiple sequence alignment → MSA
- If you use a long term frequently “phylogenetic placement of query sequences” find a shorter one “henceforth, denoted as 'query placement' “

Writing papers

- Don't use qualitative terms like “very, highly, significantly (in the non-statistical sense), much, good, bad” quantify everything as much as you can
- I personally don't like the passive form, that is, write “We implemented a cool software” instead of “a cool software has been implemented”
- “cool” shouldn't be used of course
- This also makes it much clearer what your own contribution was and what has be done by others/what is prior knowledge & work

Writing papers

- Before handing in your reports/papers use an academic “writing checker” that catches the most common mistakes!
- Academic-Writing-Check: https://github.com/devd/Academic-Writing-Check
- Make sure you know what you are doing with Latex!
- **Please read these pages!**
  - http://www.ece.ucdavis.edu/~jowens/commonerrors.html
  - http://www.cs.columbia.edu/~hgs/etc/writing-bugs.html
  - http://www.you-can-teach-writing.com/grammar_websites.html
- Attend a scientific writing course → it's worth it!

Google Scholar

- Attention when importing .bib entries from Google Scholar
- Don't just copy & paste
- You need to check the entries
  - All data available?
  - Correct Journal/Conference Abbreviations
  - Entries missing?
- I will check the reports for correct bibliography data!