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Rust Programming for HPC

Project Results

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HPC and Programming Languages

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Programming Language Characteristics

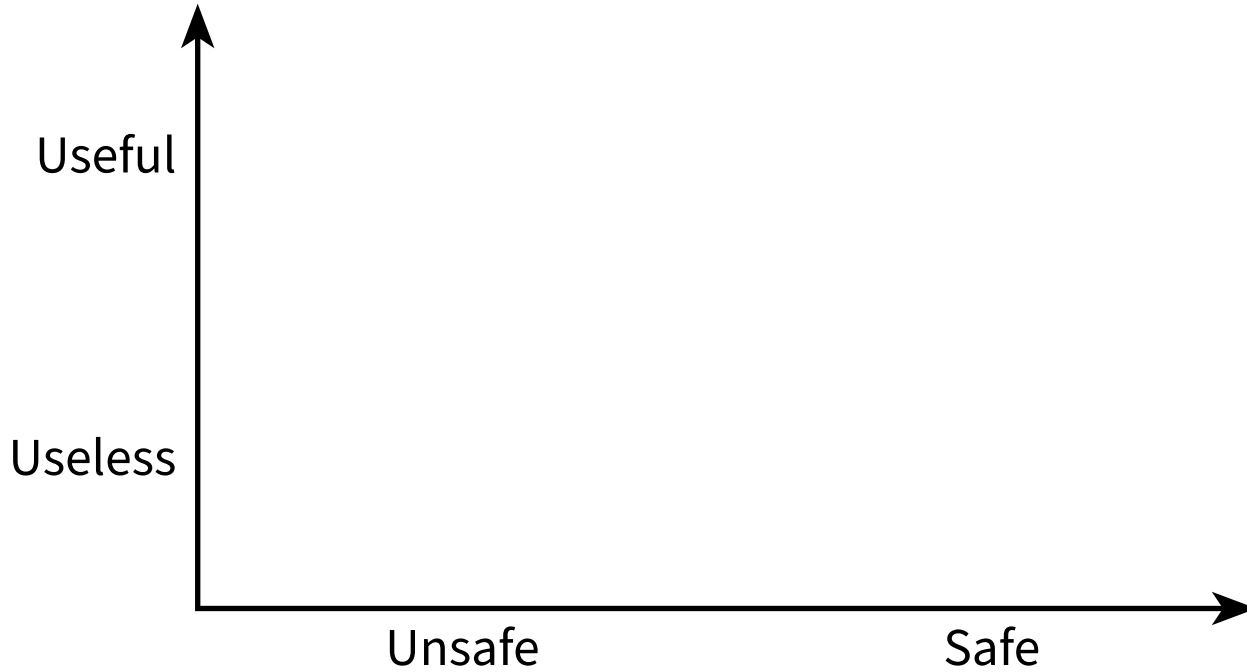
- Large number of aspects that characterize programming languages
- Examples: **Usefulness** and **Safety** [1]
- Usefulness: Performant and efficient resulting machine code, real-world applicability
- Safety: Robustness to bugs and failures



Simon Peyton Jones

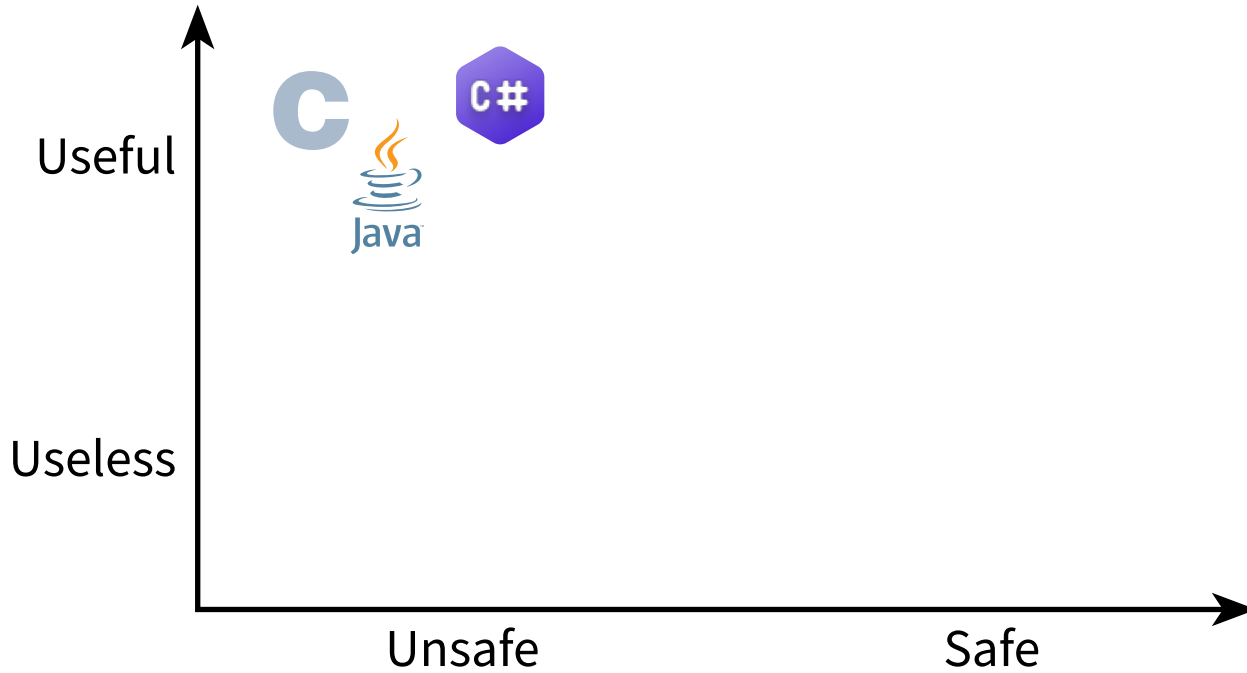
Source: [2]

Big Picture of Programming Languages



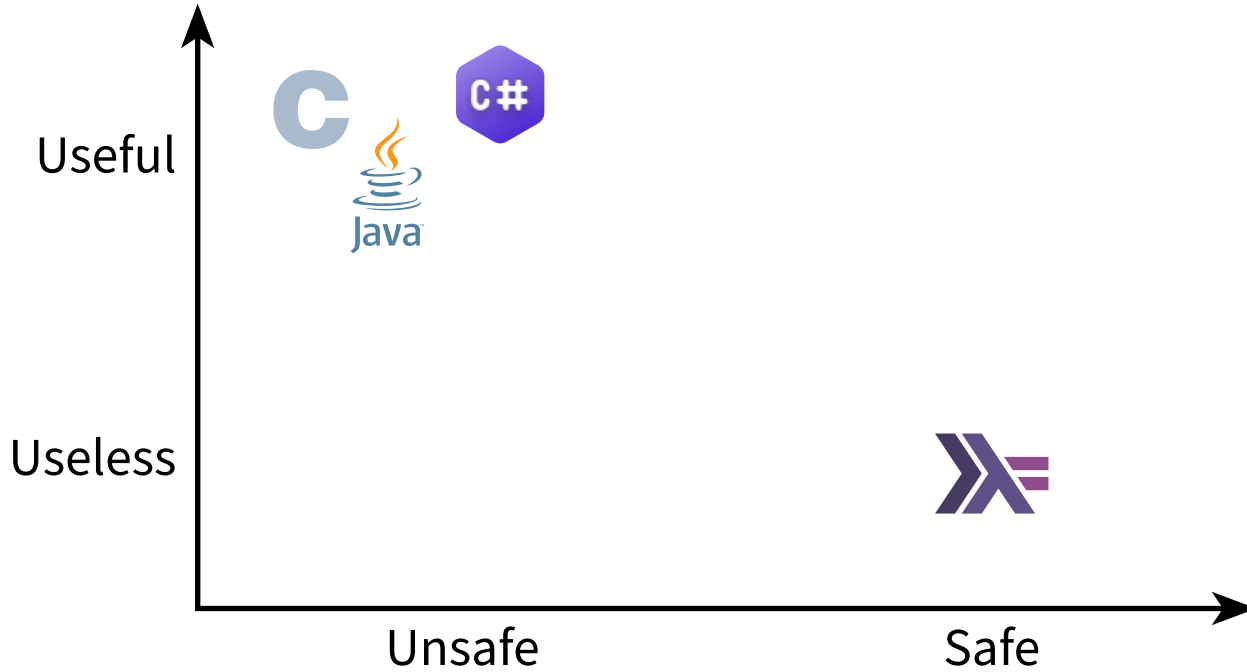
Adapted from [1], icons from [3]–[6]

Big Picture of Programming Languages



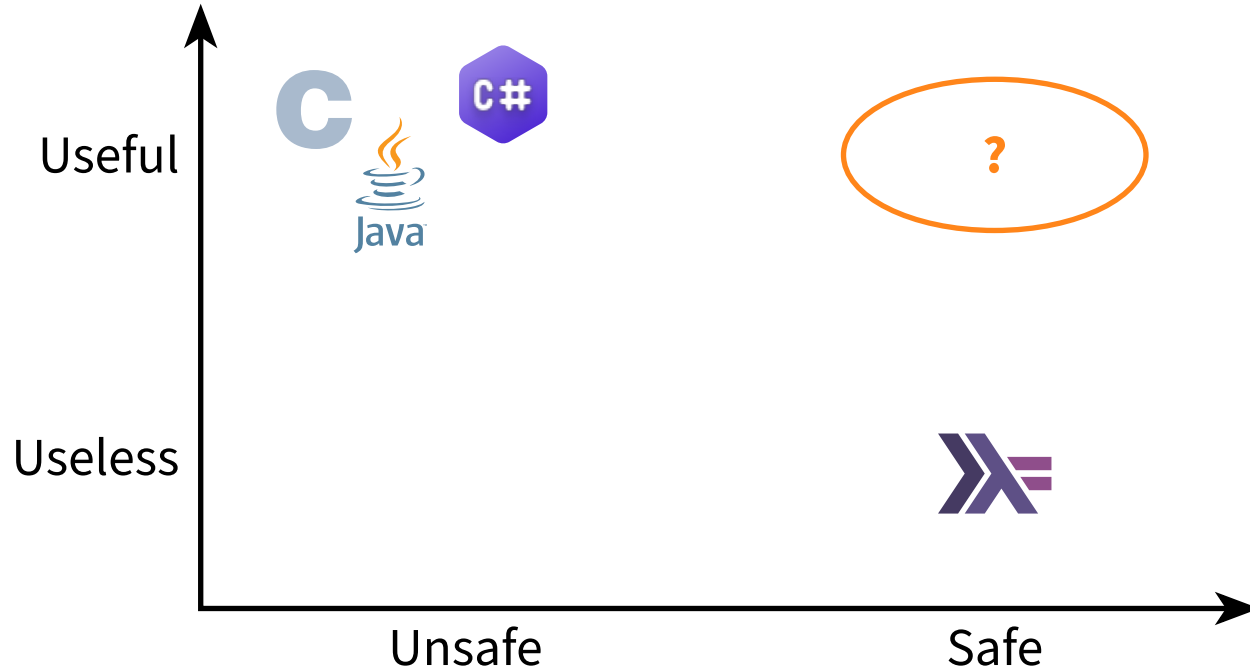
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Big Picture of Programming Languages



Adapted from [1], icons from [3]–[6]

Big Picture of Programming Languages



Adapted from [1], icons from [3]–[6]

Relevance for HPC

- Goal of high-performance computing:
 - Maximize computational power → solve computational problems as fast as possible [7]
- Enabled by software with optimal
 - Performance
 - Efficiency
 - Robustness
- Enabled by programming languages with optimal
 - Usefulness
 - Safety

The Project

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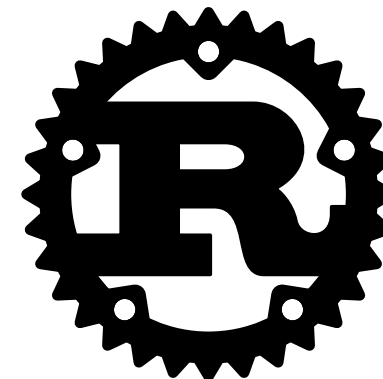
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Current HPC Programming Languages

- Currently widely used languages in HPC are not perfect
 - Cutbacks in performance, safety, ...
- Example: C
 - Performance at the cost of safety
 - E.g. memory safety and robustness
- An alternative for HPC that values the described requirements could be valuable

Rust

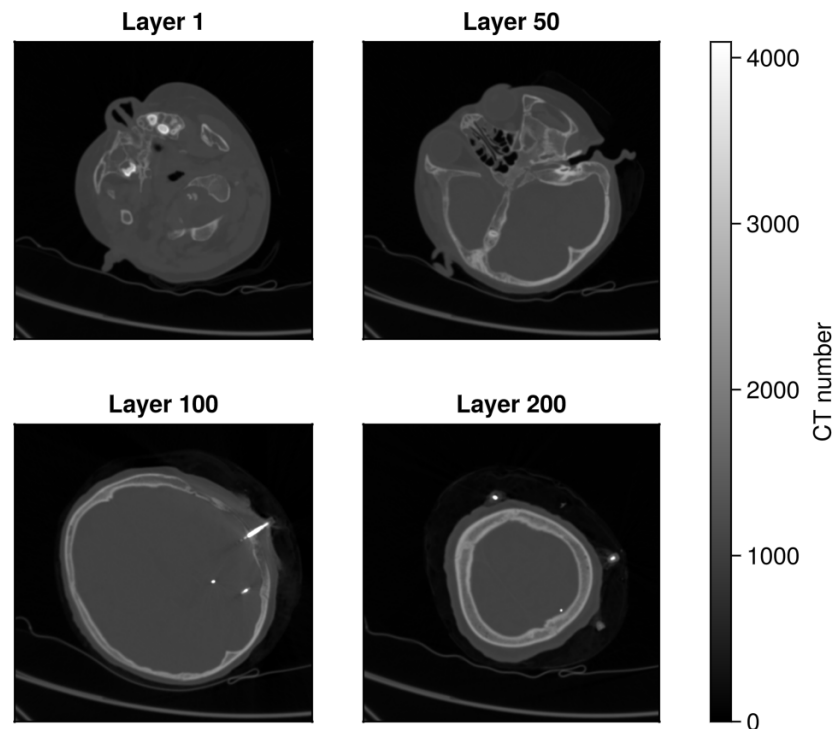
- Started in 2006, first stable release in 2015
- Now adopted by leading software companies, e.g. Google, Amazon and Microsoft [8]–[10]
- Since 2022 third supported language in Linux kernel development [11]
- Main goals: **Performance**, **Reliability** and **Productivity** [12]



⇒ **A viable alternative?**

Practical Study

- Marching Cubes Algorithm: Three-dimensional field and iso value to surface mesh
 - Implement in C and Rust
- ⇒ Compare both versions, identify Rust's capabilities and evaluate Rust for HPC programming



Data from [13]

Rust for HPC

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Rust: General Characteristics

- C-like syntax
- Imperative with declarative features
- Focus on system level while providing high-level features
- Compiled to native machine code, linked statically by default

Syntax

Euclidean distance implemented in C

```
1 #include <stdio.h>
2 #include <math.h>
3
4 int main() {
5     int vec_a[] = {1, 2, 3};
6     int vec_b[] = {4, 5, 6};
7
8     int squared_sum = 0;
9     for (int i = 0; i < 3; i++) {
10         squared_sum += pow((vec_a[i] - vec_b[i]), 2);
11     }
12
13     double eucl_distance = sqrt(squared_sum);
14     printf("Result: %f", eucl_distance);
15
16     return 0;
17 }
```


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```

Euclidean distance implemented in Rust

```
1
2
3
4 fn main() {
5     let vec_a: [i32; 3] = [1, 2, 3];
6     let vec_b = [4, 5, 6];
7
8     let mut squared_sum = 0;
9     for (x1, x2) in vec_a.into_iter().zip(vec_b) {
10         squared_sum += (x1 - x2).pow(2)
11     }
12
13     let eucl_distance = (squared_sum as f64).sqrt();
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Euclidean distance implemented in **Rust**

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Euclidean distance implemented in C

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Euclidean distance implemented in Rust

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Syntax: HPC Relevance

Advantages	Disadvantages
<ul style="list-style-type: none">• Easy to learn for developers with C-like background• Advanced syntax features, e.g. string interpolation, improve readability and maintainability of source code	<ul style="list-style-type: none">• Can get complicated and confusing

- Relevance for HPC:
 - Increased productivity, easy to learn, increased maintainability

Semantics: Declarative Features

```
1 let mut intersection_index = 0;
2 for (i, value) in cube.values.iter().enumerate() {
3     if (*value as f32) < iso_value {
4         intersection_index |= 1 << i;
5     }
6 }
```

Iteration in Rust using for-loop

```
1 let intersection_index = cube
2   .values
3   .iter()
4   .enumerate()
5   .filter(|(_, v)| v < iso_value)
6   .map(|(i, _)| i)
7   .reduce(|acc, e| acc | (1 << e));
```

Iteration in Rust using reactive constructs

Semantics: Advanced Typing

```
1 #[derive(Debug)]
2 pub enum NpyError {
3     OpenFileError(io::Error),
4     MissingMagicString,
5     UnexpectedNumberOfBytesRead(usize, usize),
6 }
7
8 impl From<io::Error> for NpyError {
9     fn from(value: io::Error) -> Self {
10         NpyError::OpenFileError(value)
11     }
12 }
```

Enums and methods in Rust

```
1 pub struct NpyArray<T, D>
2 where
3     D: Dimension,
4     T: NpyType,
5 {
6     pub version_major: u8,
7     pub version_minor: u8,
8     pub header: Header<T>,
9     pub data: Array<T::Inner, D>,
10 }
11
12 fn main() {
13     let data: NpyArray<NpyLeI2, Ix3>
14         = NpyArray::read(conf.input);
15 }
```

Structs and generics in Rust

Semantics: Memory Safety

- **Ownership:** Special set of rules governing Rust code
- Enforced by compiler
 - Type-safety at compile time
 - Can be overridden manually if required
- Enhances memory safety drastically and prevents memory bugs, e.g.
 - Memory leaks
 - Dangling pointers
 - Double frees

Semantics: HPC Relevance

Advantages	Disadvantages
<ul style="list-style-type: none">• Safety with very little to no performance penalty• Comprehensive standard library for e.g. declarative programming• Excellent type system and extensibility	<ul style="list-style-type: none">• Ownership system is unique; steep learning curve• Enforced safety may be exhaustive and unnecessary at points• Cost of higher-level features not always transparent

- Relevance for HPC:
 - Increased productivity and maintainability, safety for little to no overhead, extensibility
 - Cost of certain features and abstractions have to be considered

HPC Ecosystem

- Classic HPC paradigms and technologies:
 - Parallel computations with shared memory, e.g. OpenMP
 - Distributed computing with distributed memory, e.g. MPI
 - Rust’s capabilities?
- Rust’s semantics enable “fearless concurrency”
 - Comprehensive parallel computing support in standard library
 - Native thread support
 - Mutexes, reference counter, channels, etc.
 - Without sacrificing safety
 - Support for asynchronous programming

Rayon

- But: Like in e.g. C, manual threading for data parallelism can be exhaustive
→ Simple using OpenMP
- Rust's solution: *Rayon* [14]
 - Library for data parallelism
 - Uses Rust's declarative features and constructs for high-level data parallelism

```
1 let triangles: Vec<Triangle>
2   = Zip::from(indices(indices_shape))
3     .into_par_iter()
4     .flat_map(|((i, j, k),)| {
5         // [...]
6         triangulate_cube(&cube, iso_value)
7     })
8     .collect();
```

Usage example of Rayon

Distributed Computing with Rust?

- At the time of writing, limited options exist for distributed computing using Rust
- Few native Rust solutions
 - Example: *constellation* [15]
- Like for many other languages, e.g. MPI bindings exist [16]
 - Bindings to given C implementation of MPI
 - Abstracts away “unsafe” C code
 - Provides Rust abstractions and higher-level constructs
 - Evaluation is out of scope for this project

Rust Ecosystem: HPC Relevance

Advantages	Disadvantages
<ul style="list-style-type: none">• Good support for concurrent and parallel programming• Safety implied by Rust's semantics• Vast standard library, well-supported external libraries	<ul style="list-style-type: none">• Limited support for distributed computing

- Relevance for HPC:
 - Safe concurrency and parallelism with little effort
 - May be unsuited for distributed workloads

Implementation Results

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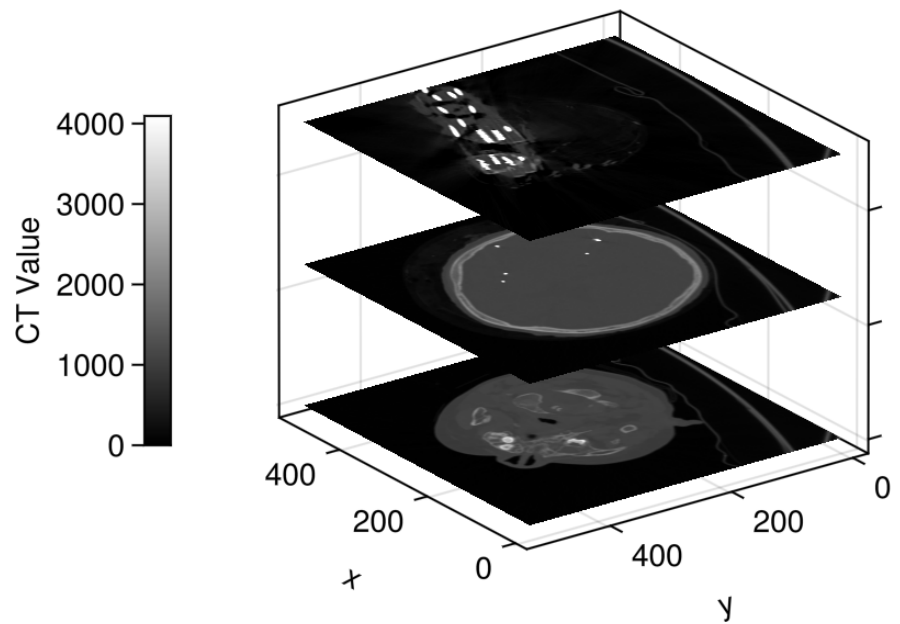
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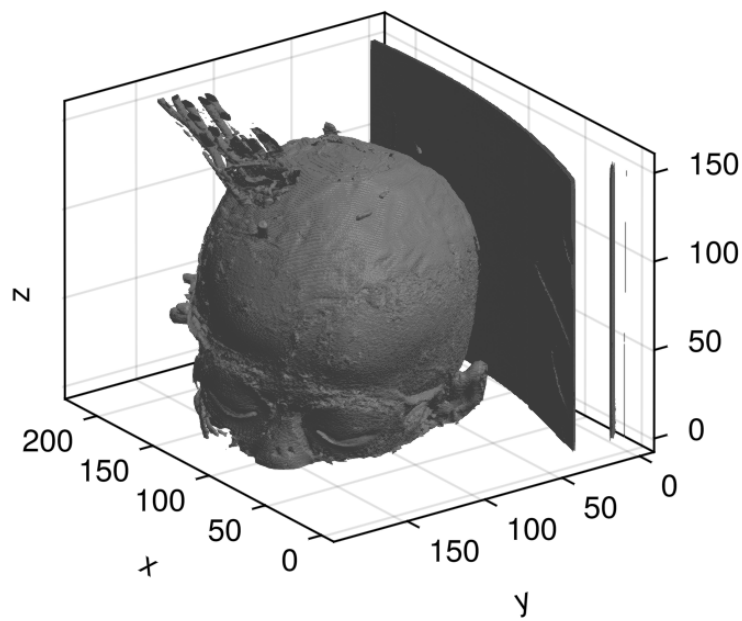
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Functional Results

Layers in Volumetric Data



Resulting Mesh for $v = 1500$



Data from [13]

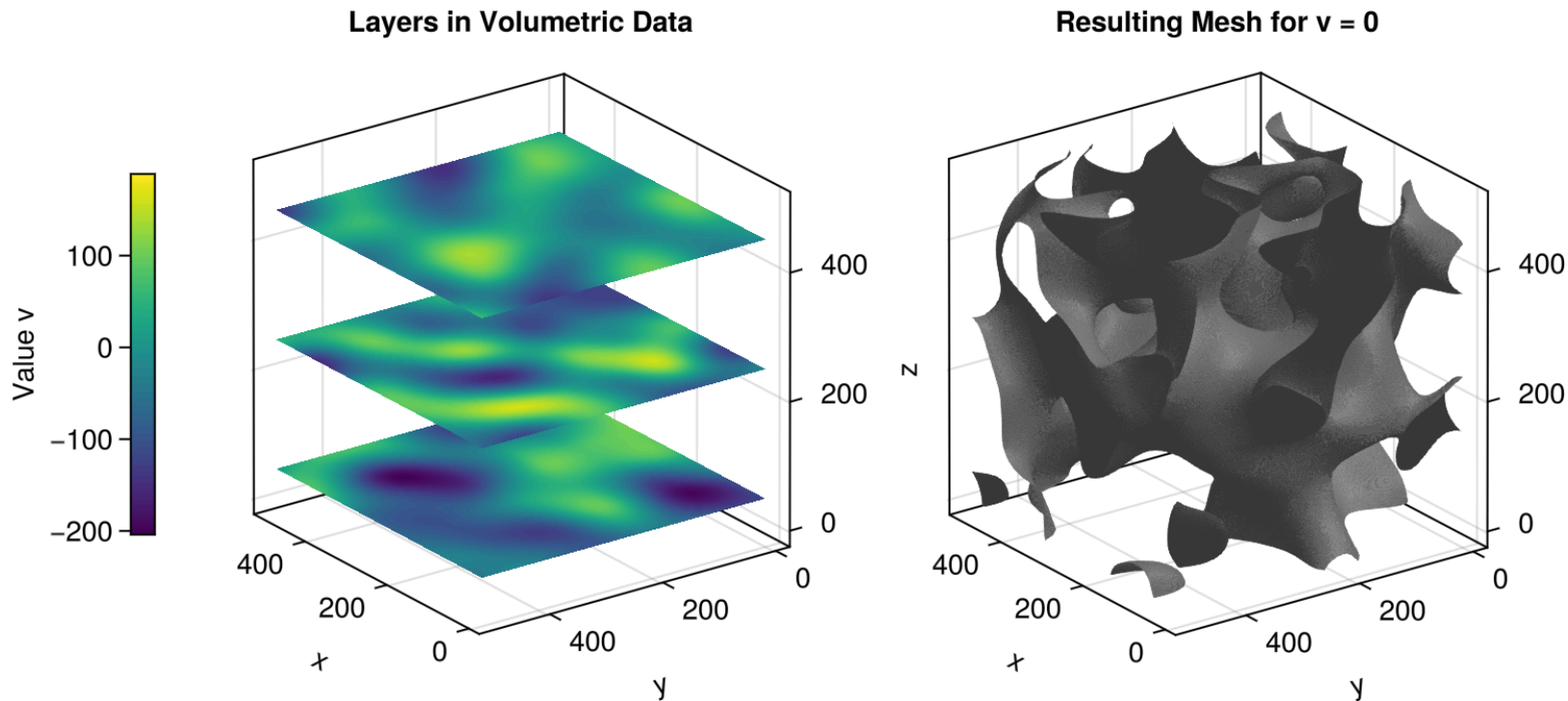
Implementation Details

- Goal of implementing Marching Cubes in C as well as Rust:
 - Gain insights about Rust's capabilities
 - Get overview of Rust's performance compared to established HPC language
- Both implementations function in the same way
 - Two versions each: sequential and parallel (shared memory)
 - Rust version offers several enhancement using Rust-specific features, e.g.
 - Extensible typing
 - Error handling
 - Different data representation in memory

Benchmarking Process

- One benchmark for wall-clock time of the sequential version
- One benchmark for analyzing strong-scaling behaviour of the parallel version

Benchmark Data



Data generated using [17]

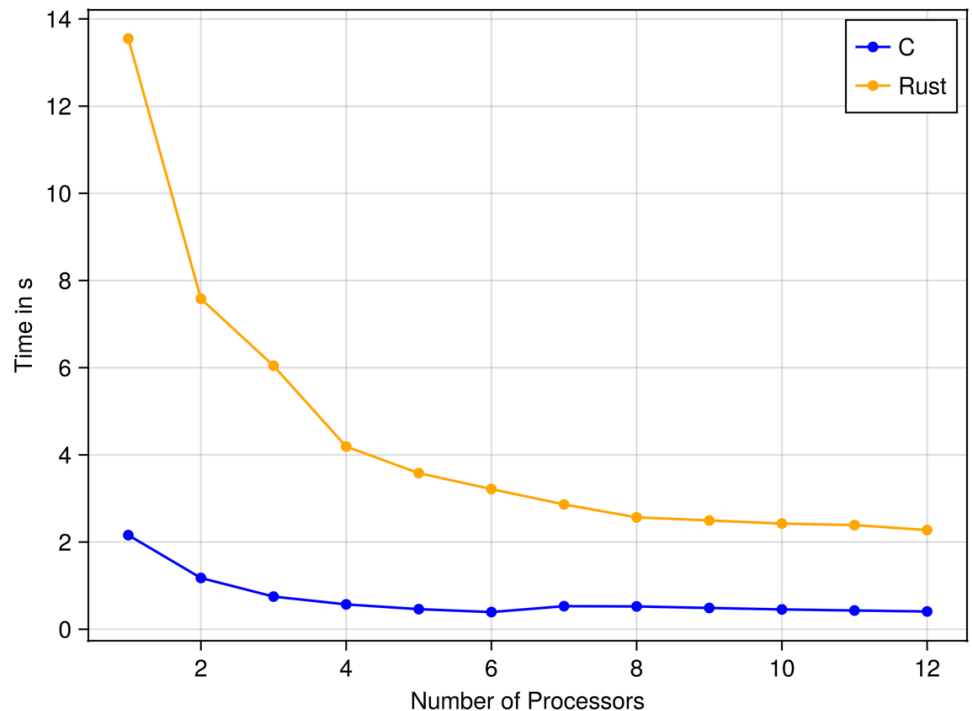
Benchmark Results: Sequential

Implementation	μ	σ	Range
C	2.11 s	0.02	2.09 s – 2.19 s
Rust	6.55 s	0.03	6.53 s – 6.63 s

Time needed for executing the algorithm

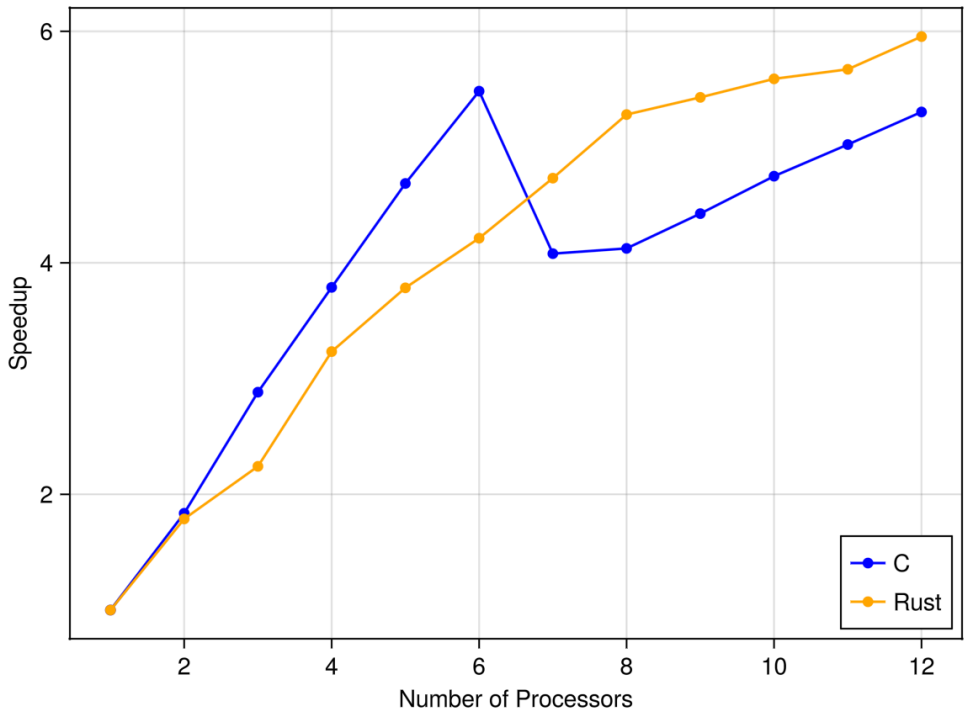
Executed on a Gigabyte AERO 15XV8 with an Intel Core i7-8750H CPU
(4.10 GHz, 12 threads) and DDR4 RAM (16GB, 2667 MT/s), 20 iterations executed

Benchmark Results: Parallel



Runtime of the parallel version, depending on the number of processors used

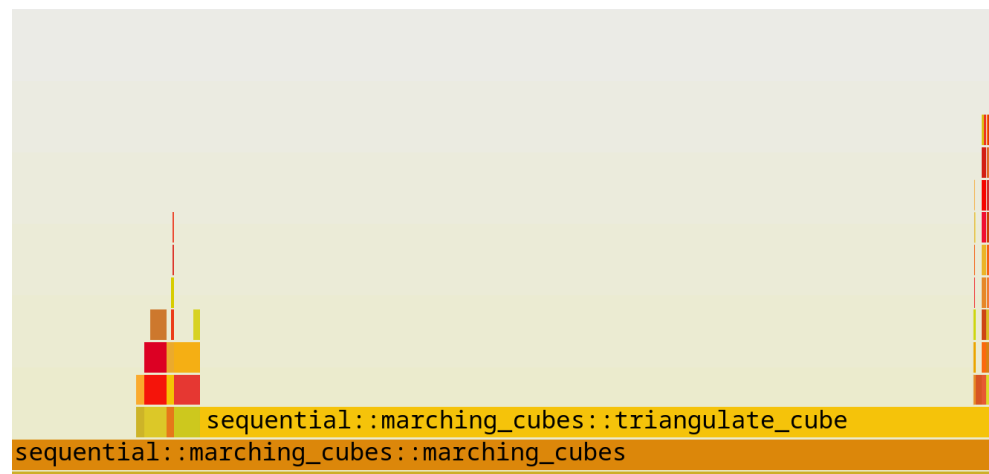
Benchmark Results: Parallel



Speedup of the parallel version

Benchmark Analysis

- Results contradict expectations set by Rust
- Existing C debugging tools work with Rust
- Flamegraph allows analysis to some degree [18]
- Several hypotheses, no hard evidences yet



Flamegraph of the sequential version generated using [18]

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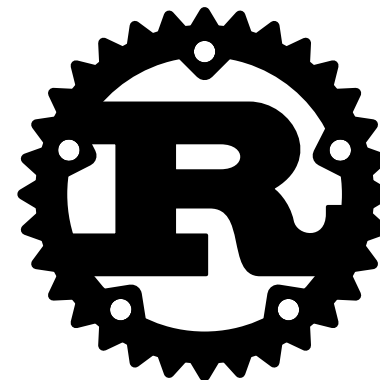
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Rust: Summary

- High maintainability
- High extensibility
- Memory safety without overhead
- Full control, e.g. over efficiency
- High performance, in theory



Outlook

- Implementations finished, first insights could be gained
 - But: Results are questionable
- Further work this semester:
 - Refine benchmarks and implementations
 - Research reasons for outcomes
- Future work:
 - Evaluate suitability for distributed workloads, e.g. bindings for MPI

Rust for HPC Programming?

- Decision of using Rust for an HPC project should be based on
 - Project requirements
 - Trade-off between advantages and disadvantages
 - People
- Mature and effective for parallel computations
 - Valuable approaches and solutions that HPC may benefit from
- Possibly valuable for distributed HPC use cases in the future

References

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