

Marcin Copik

AXeleration as a Service (XaaS): From Batch Jobs to Elastic Services in Scientific Computing

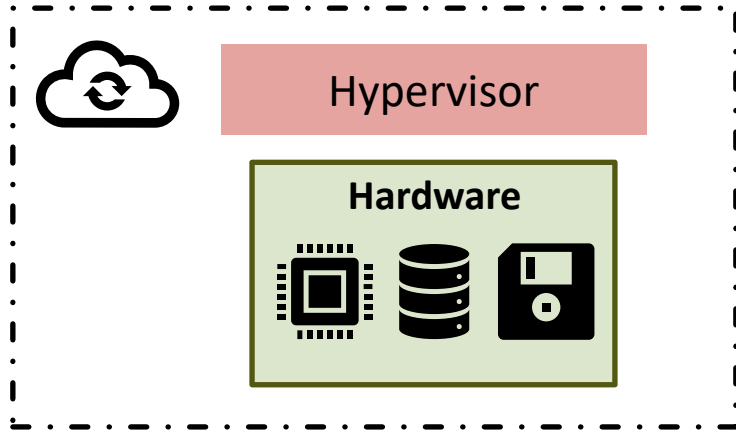


HPC·AI
ADVISORY COUNCIL
NETWORK OF EXPERTISE

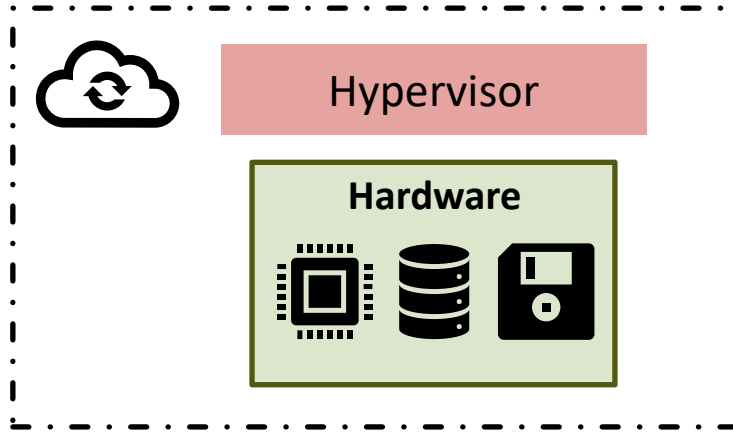
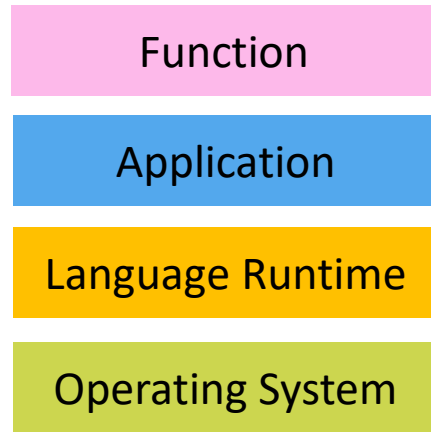
HPC-AI Swiss
Conference

Cloud Evolution

Cloud Evolution

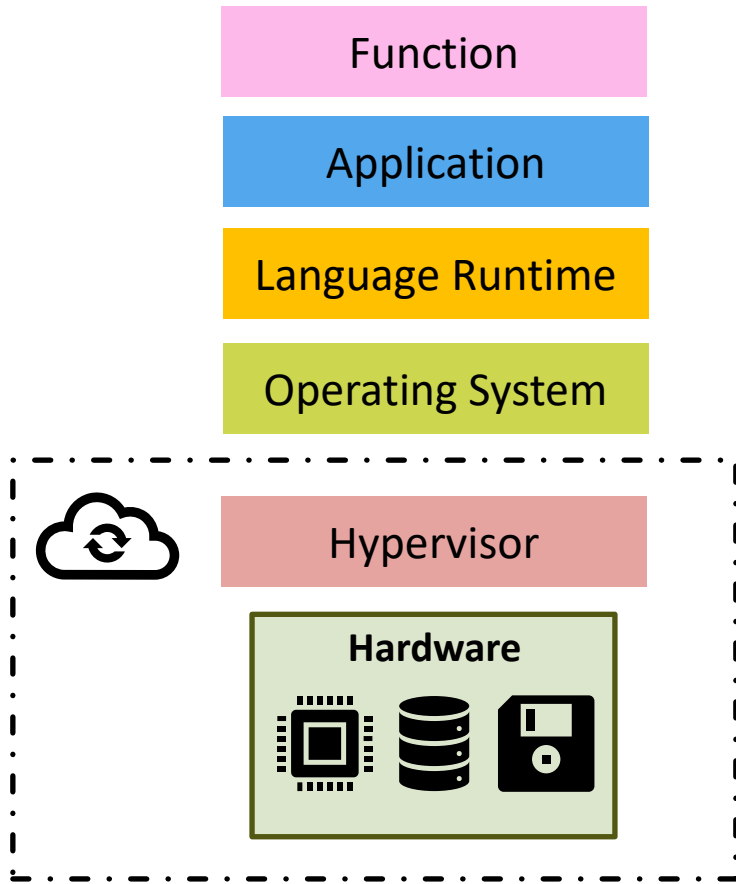


Cloud Evolution

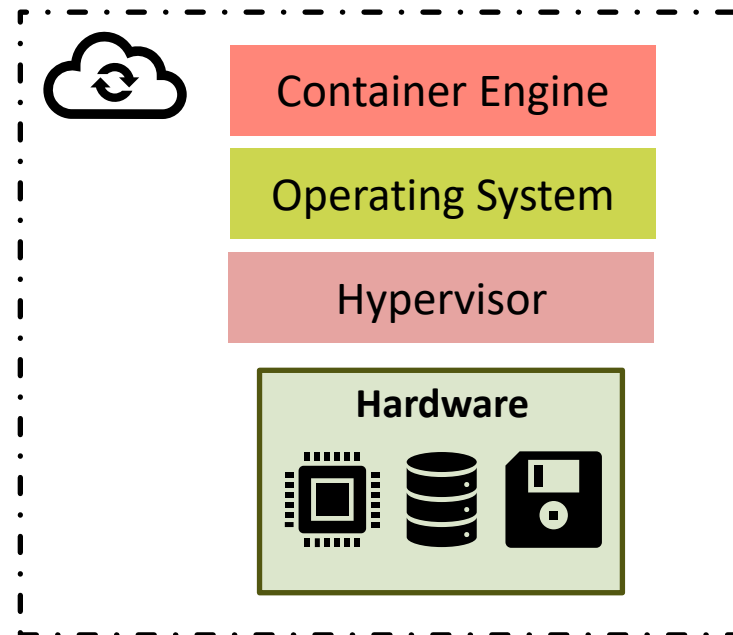


**Virtual Machine
(Infrastructure-as-a-Service)**

Cloud Evolution

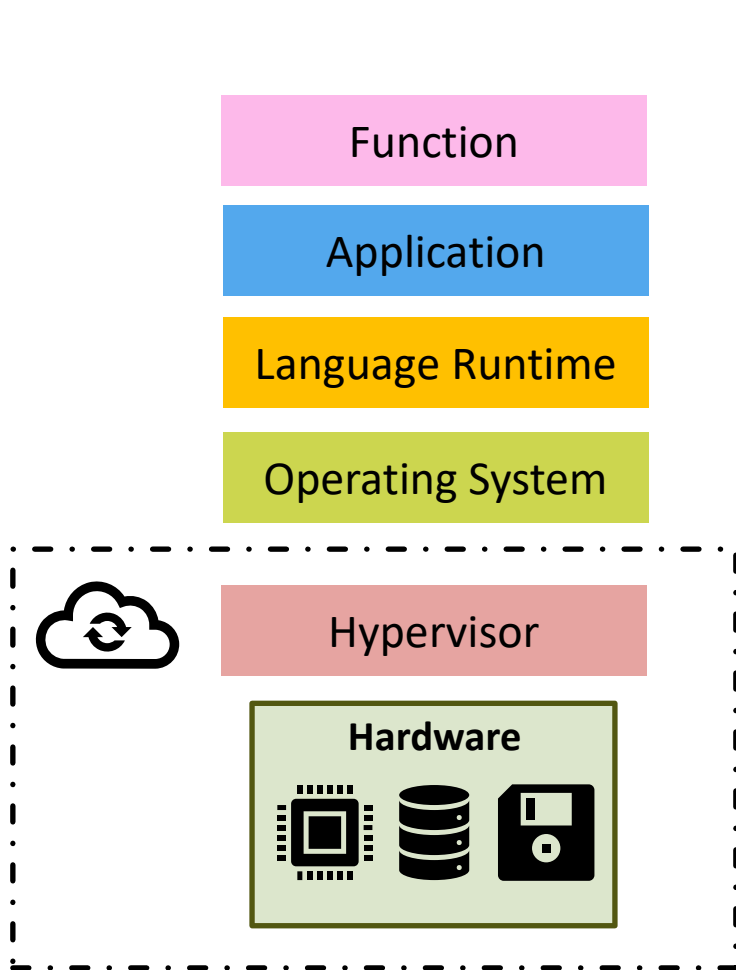


Virtual Machine
(Infrastructure-as-a-Service)

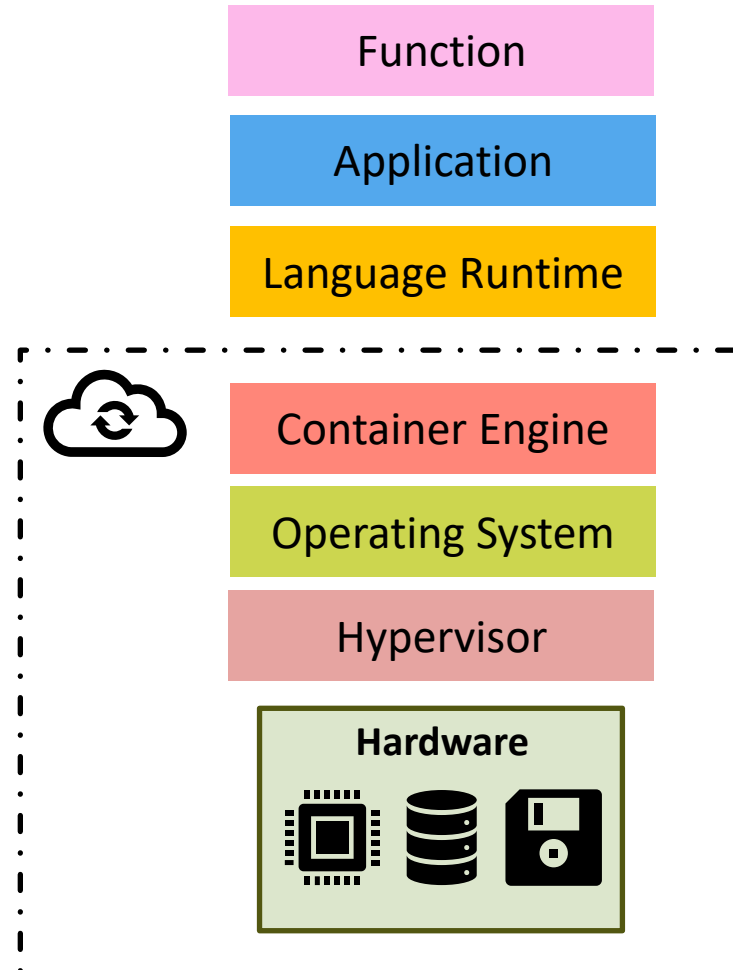


Containers
(Container-as-a-Service)

Cloud Evolution

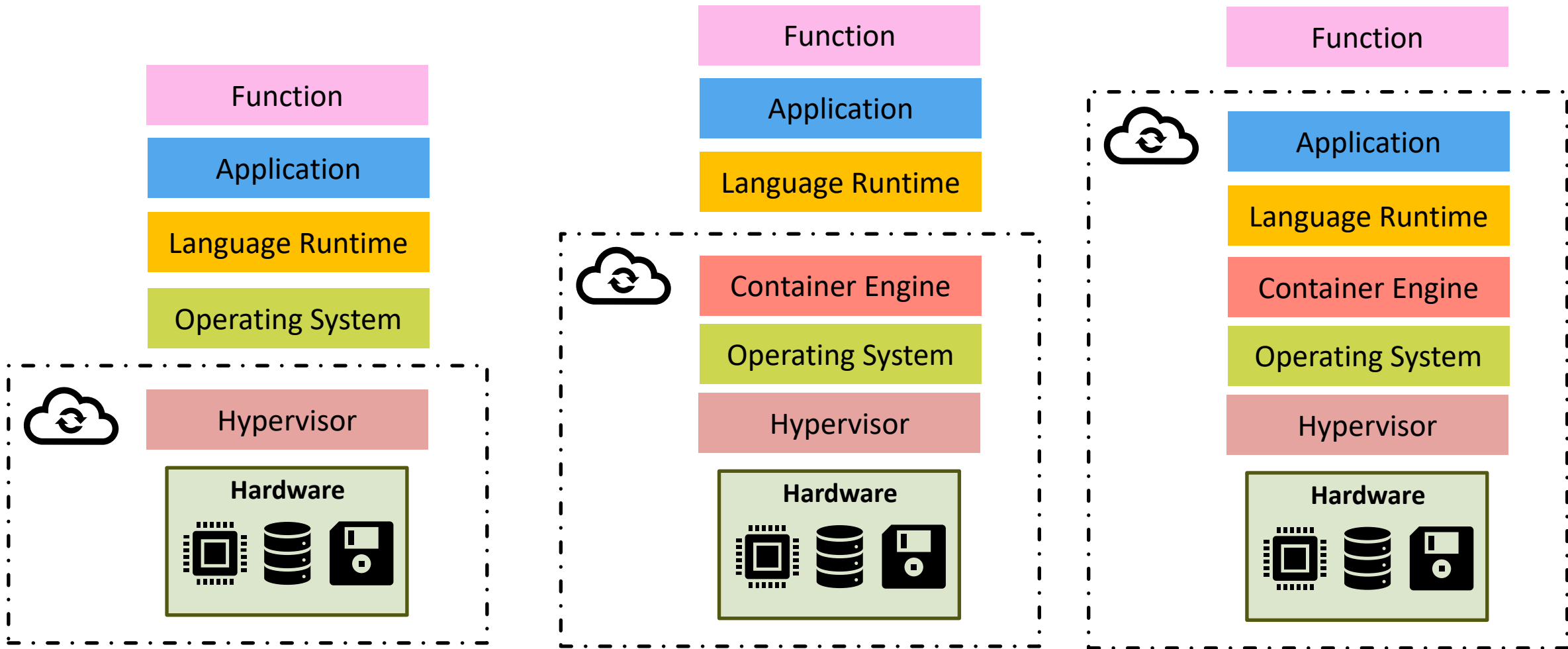


Virtual Machine
(Infrastructure-as-a-Service)



Containers
(Container-as-a-Service)

Cloud Evolution



Virtual Machine
(Infrastructure-as-a-Service)

Containers
(Container-as-a-Service)

Functions
(Function-as-a-Service)

Function-as-a-Service (FaaS): Good and Bad

```
model = model_init(cloud_storage, 'resnet50')
```

```
def handler_function(request: dict, context: dict):
```

```
    data = cloud_storage.read(request['id'])
```

```
    result = inference(request['op'], data)
```

```
    return result
```

Function-as-a-Service (FaaS): Good and Bad

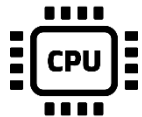



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Configuration: ⁺    

Function-as-a-Service (FaaS): Good and Bad

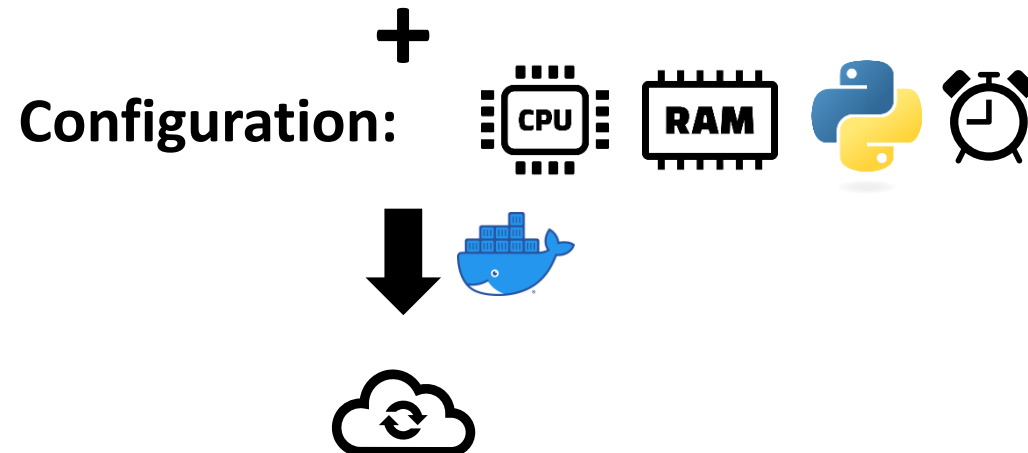
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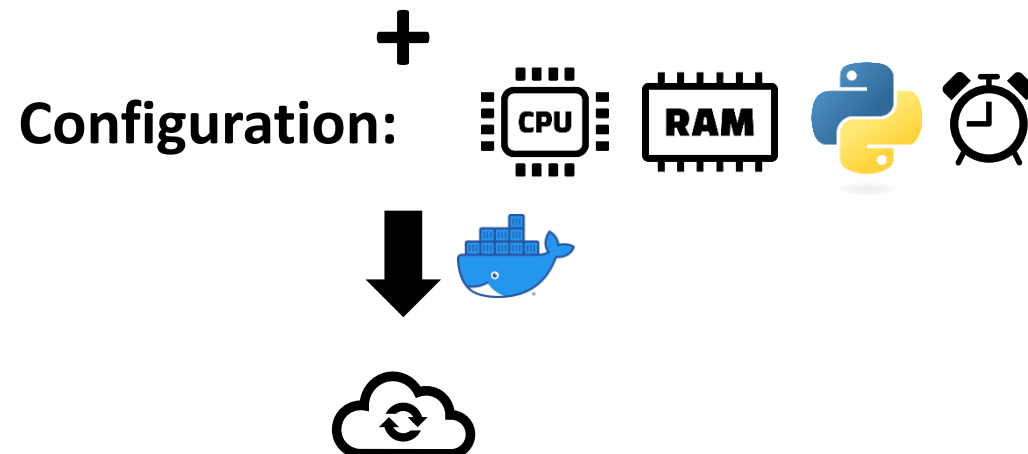
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No Infrastructure Management

Elastic Jobs

Improved Utilization

Fast Scalability



Function-as-a-Service (FaaS): Good and Bad

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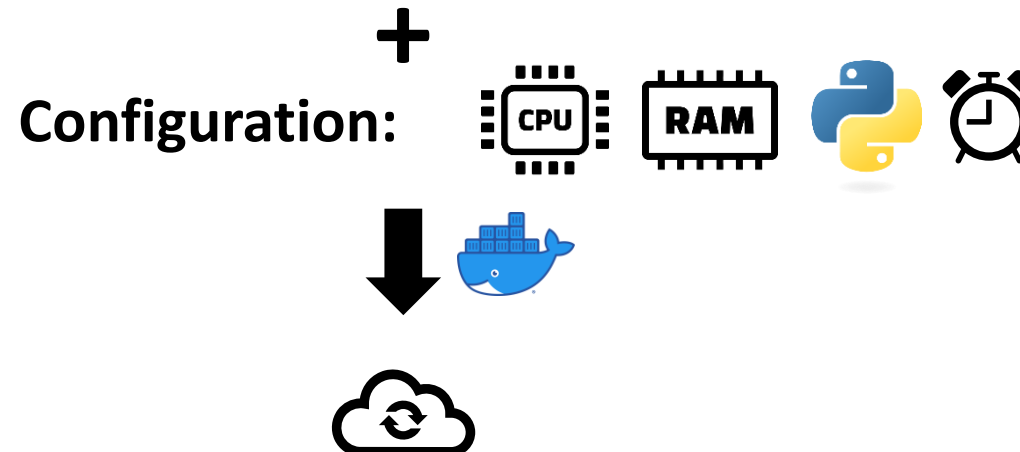
Fast Scalability

Disaggregated Compute from Storage

“Stateless” Functions

No Infrastructure Management

Black Box System



Serverless Was Not Designed for HPC...

AWS Lambda turns 10: A rare look at the doc that started it

November 14, 2024 • 5460 words

Serverless Was Not Designed for HPC...

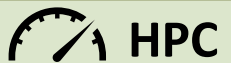
31. How does Lambda support parallel processing?

*Developers can run multiple applications and/or **multiple copies of the same application simultaneously**. They can also access Lambda APIs programmatically from within applications, using the AWS client SDK, which allows them to delegate and orchestrate work by running other applications.*

Serverless Was Not Designed for HPC...

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Burst Launches, Colocation Policies
Bulk Synchronous Parallel Model
Communicators, Message Passing, Collectives

...

Serverless Was Not Designed for HPC...

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Burst Launches, Colocation Policies
Bulk Synchronous Parallel Model
Communicators, Message Passing, Collectives
 ...



Embarrassingly Parallel

...But Science Adapted It Anyway

FAASTLOOP: Optimizing Loop-Based Applications for Serverless Computing

Occupy the Cloud: Distributed Computing for the 99%

Eric Jonas, Oifan Pu, Shivaram Venkataraman, Ion Stoica, Benjamin Recht

Burst Computing: Quick, Sudden, Massively Parallel Processing on Serverless Resources

Daniel Barcelona-Por
Center; Aitor Arjo
Step

funcX: A Federated Function Serving Fabric for Science

Ryan Chard
Argonne National Laboratory

Yadu Babuji
University of Chicago

Zhuozhao Li
University of Chicago

Tyler Skluzacek
University of Chicago

Anna Woodard
University of Chicago

Ben Blaiszik
University of Chicago

Ian Foster
Argonne National Laboratory and
University of Chicago

Kyle Chard
University of Chicago and Argonne
National Laboratory

...But Science Adapted It Anyway

Serverless execution of scientific workflows: Experiments with HyperFlow, AWS Lambda and Google Cloud Functions

Maciej Malawski *, Adam Gajek, Adam Zima, Bartosz Balis, Kamil Figiela

AGH Univer

DayDream: Executing Dynamic Scientific Workflows on Serverless Platforms with Hot Starts

Rohan Basu Roy
Northeastern University
Boston, MA, USA

Tirthak Patel
Northeastern University
Boston, MA, USA

Devesh Tiwari
Northeastern University
Boston, MA, USA

Mashup: Making Serverless Computing Useful for HPC Workflows via Hybrid Execution

Rohan Basu Roy
Northeastern University

Vijay Gadepally
MIT Lincoln Laboratory

Tirthak Patel
Northeastern University

Devesh Tiwari
Northeastern University

Zhuozhao Li
University of Chicago

Ben Blaiszik
University of Chicago

and Argonne
Laboratory

SOFTWARE

Democratising high performance computing for bioinformatics through serverless cloud computing: A case study on CRISPR-Cas9 guide RNA design with Crackling Cloud

Jacob Bradford^{1,2*}, Divya Joy¹, Mattias Winsen¹, Nicholas Mackenzie Wilkins¹, Laurence O.W. Wilson^{3,4}, Denis C. I.

Flows: Experiments with
Cloud Functions
sz Balis, Kamil Figiela

A Serverless Engine for High Energy Physics Distributed Analysis

1st Jacek Kuśnierz
Institute of Computer Science
AGH
Kraków, Poland

2nd Vincenzo E. Padulano
EP-SFT, CERN
Geneva, Switzerland
DSIC LLPV

3rd Maciej Malawski
Institute of Computer Science
AGH
Kraków, Poland

4th Kamil Burkiewicz
Institute of Computer Science
AGH
Kraków, Poland

A serverless computing architecture for Martian aurora detection with the Emirates Mars Mission

[David Pacios](#), [José Luis Vázquez-Poletti](#) ✉, [Dattaraj B. Dhuri](#), [Dimitra Atri](#), [Rafael Moreno-Vozmediano](#),

[Robert J. Lillis](#), [Nikolaos Schetakis](#), [Jorge Gómez-Sanz](#), [Alessio Di Iorio](#) & [Luis Vázquez](#)

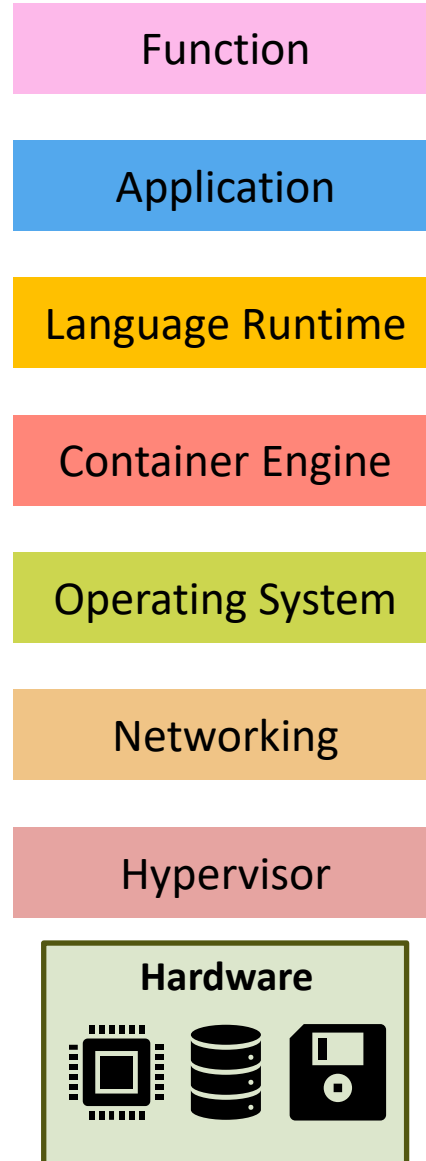
[Scientific Reports](#) **14**, Article number: 3029 (2024) | [Cite this article](#)

8th Valentina Avati
EP-UHC
CERN
Geneva, Switzerland

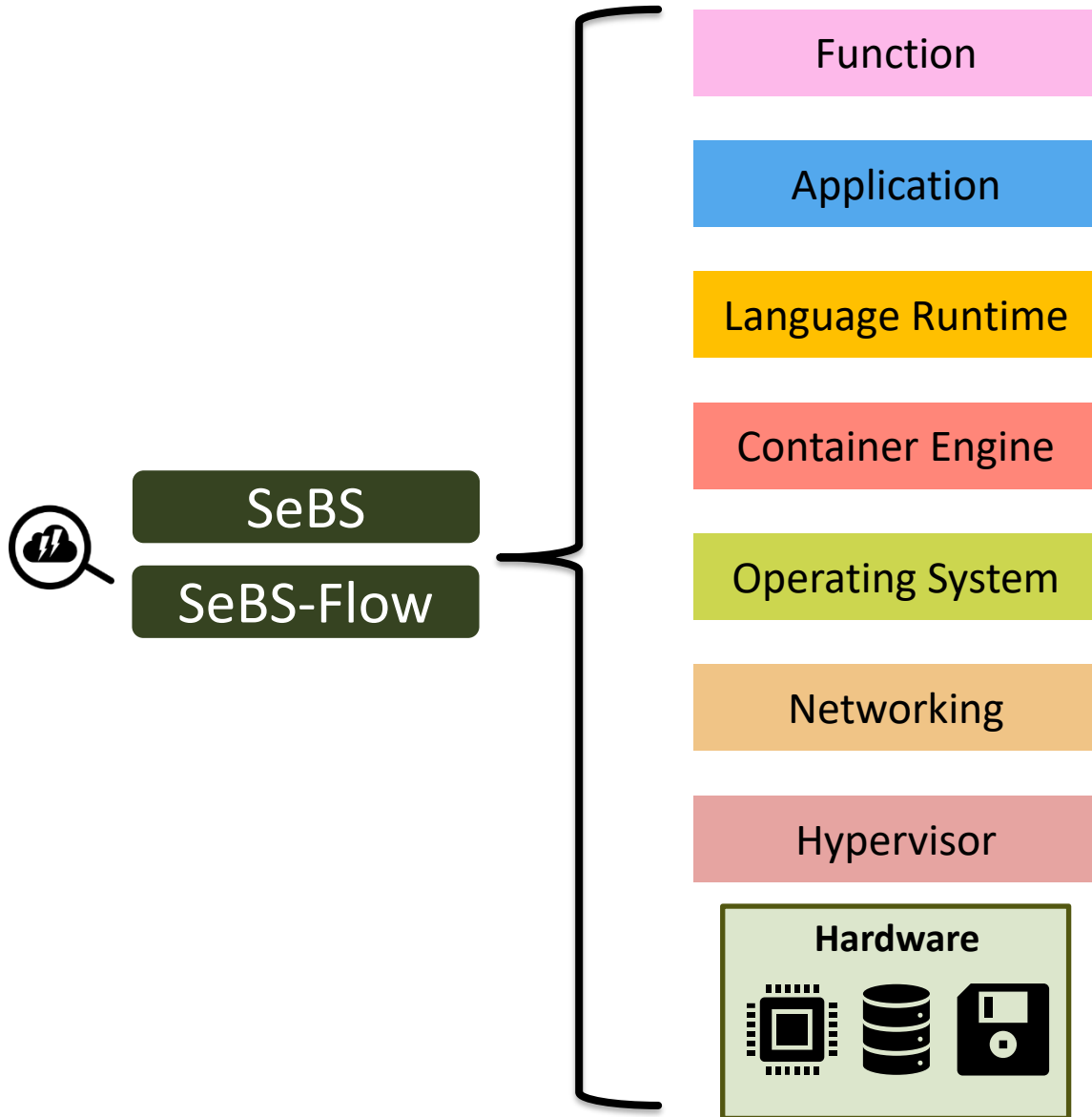
Ben Blaiszik
University of Chicago

rd
and Argonne
atory

AXelerating Serverless Computing: Measure!



AXelerating Serverless Computing: Measure!



SeBS: The Serverless Benchmark Suite

 [spcl/serverless-benchmarks](https://github.com/spcl/serverless-benchmarks)



“SeBS: a Serverless Benchmark Suite for Function-as-a-Service Computing”, Middleware 2021

SeBS: The Serverless Benchmark Suite

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Cloud-Agnostic



“SeBS: a Serverless Benchmark Suite for Function-as-a-Service Computing”, Middleware 2021

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Representative Benchmarks



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Cloud-Agnostic



Representative Benchmarks



Automatic Experiments

Performance & Cost
Invocation Overhead
Container Eviction
Communication



“SeBS: a Serverless Benchmark Suite for Function-as-a-Service Computing”, Middleware 2021

SeBS: The Serverless Benchmark Suite

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Representative Benchmarks

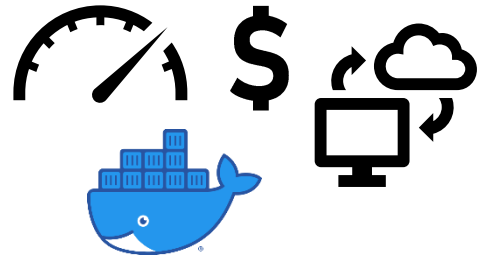


Automatic Experiments

Performance & Cost
Invocation Overhead
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Insights



“SeBS: a Serverless Benchmark Suite for Function-as-a-Service Computing”, Middleware 2021

SeBS: The Serverless Benchmark Suite

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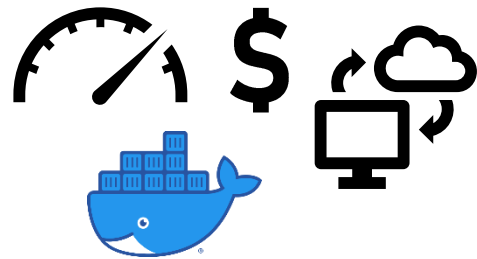
Representative Benchmarks



Automatic Experiments

Performance & Cost
Invocation Overhead
Container Eviction
Communication

Insights



Adoption & Community


99 forks
30+ contributors


Google
Summer of Code



“SeBS: a Serverless Benchmark Suite for Function-as-a-Service Computing”, Middleware 2021



SeBS: The Serverless Benchmark Suite



“Which platform is best for my workload? Can my application scale? What are the performance limits of each platform?”





SeBS: The Serverless Benchmark Suite



“Which platform is best for my workload? Can my application scale? What are the performance limits of each platform?”



Deploy with SeBS

Allocate Cloud Resources

Build Functions

Upload Data

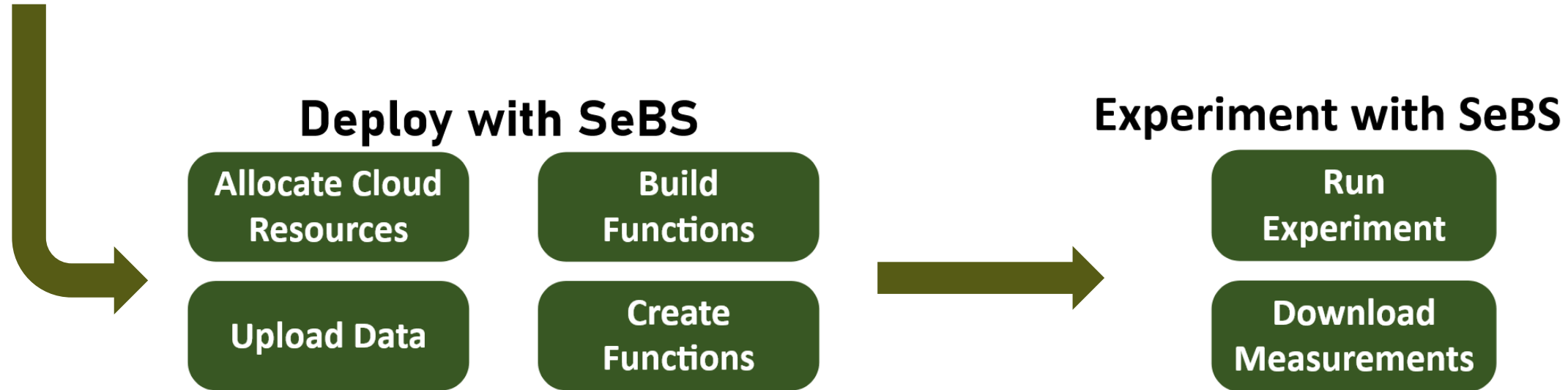
Create Functions



SeBS: The Serverless Benchmark Suite



“Which platform is best for my workload? Can my application scale? What are the performance limits of each platform?”



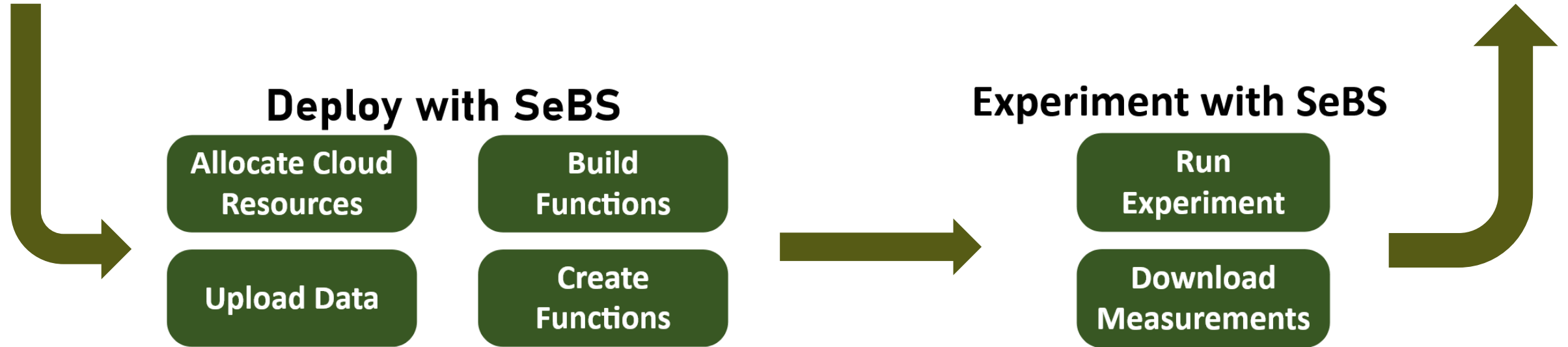
SeBS: The Serverless Benchmark Suite



“Which platform is best for my workload? Can my application scale? What are the performance limits of each platform?”



“The end-to-end latency is not what I expected because of lower scalability and variable I/O performance.”

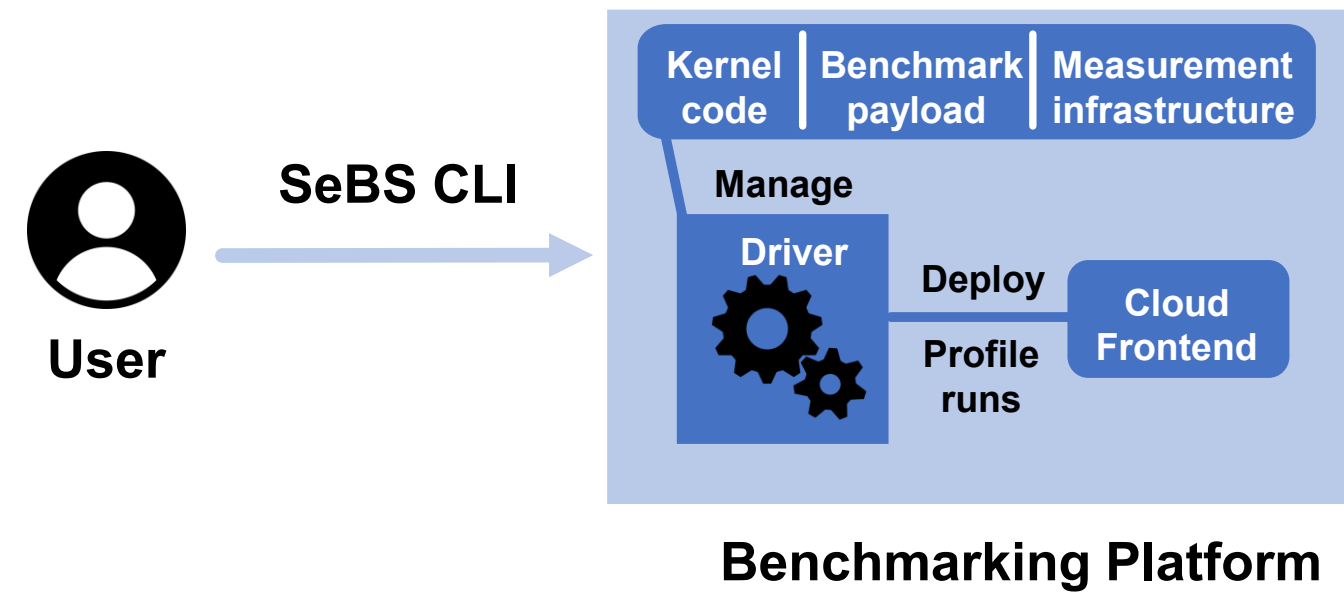


SeBS: Architecture



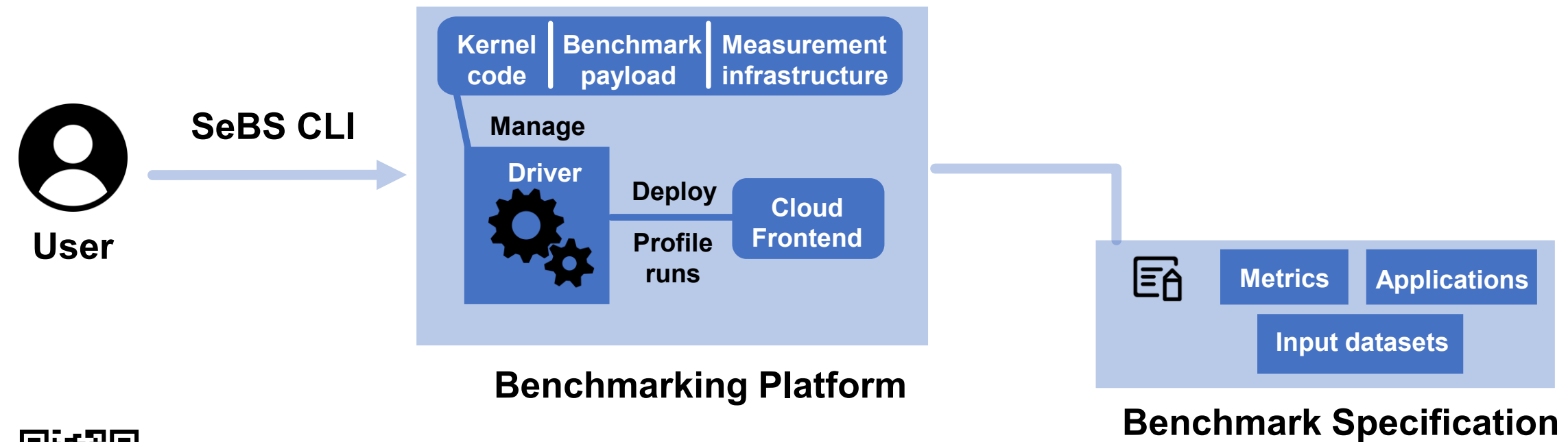
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SeBS: Architecture



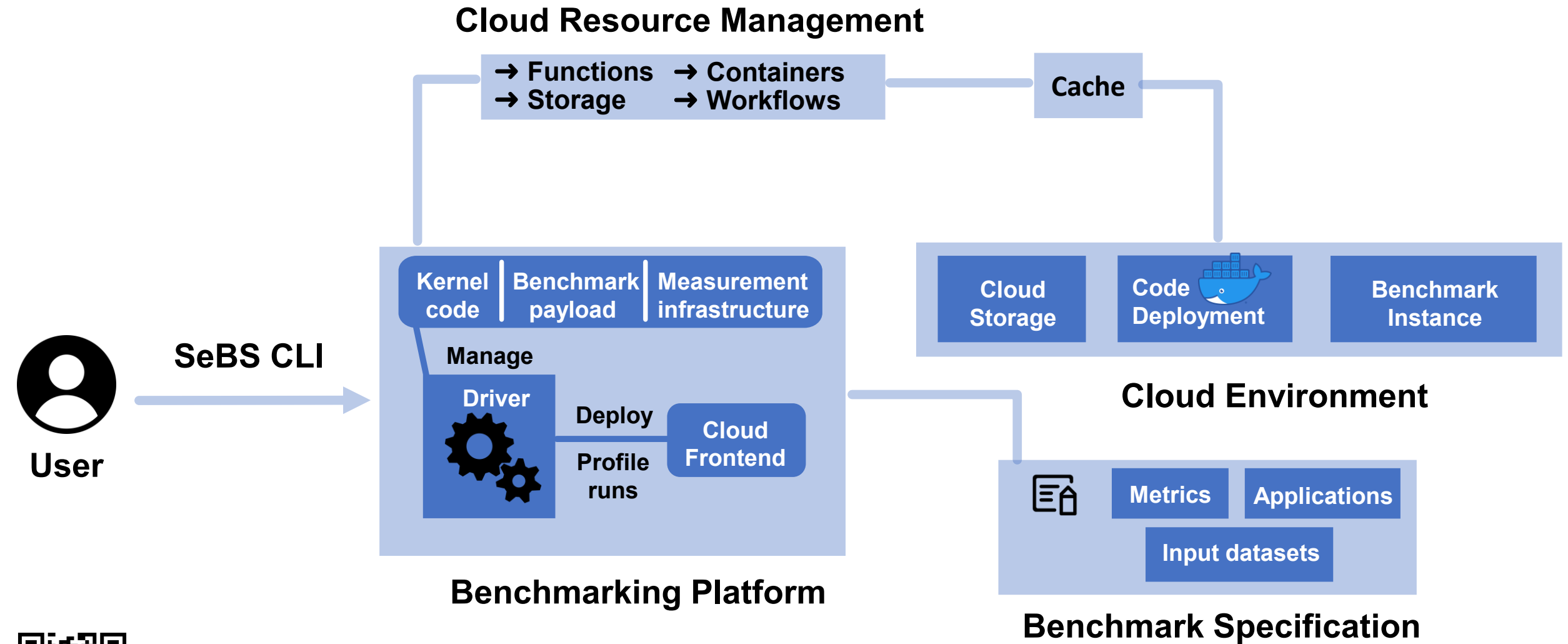
“SeBS: a Serverless Benchmark Suite for Function-as-a-Service Computing”, Middleware 2021

SeBS: Architecture



“SeBS: a Serverless Benchmark Suite for Function-as-a-Service Computing”, Middleware 2021

SeBS: Architecture



“SeBS: a Serverless Benchmark Suite for Function-as-a-Service Computing”, Middleware 2021

SeBS: Cloud Platforms



“SeBS: a Serverless Benchmark Suite for Function-as-a-Service Computing”, Middleware 2021

SeBS: Cloud Platforms



**Big Three: similar capabilities,
different semantics.**



SeBS: Cloud Platforms



**Big Three: similar capabilities,
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**Open-source FaaS, run on any
Kubernetes.**



SeBS: Cloud Platforms



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**Experimental support: see
GitHub PRs for the branch.**



SeBS: Cloud Platforms



Big Three: similar capabilities, different semantics.



Open-source FaaS, run on any Kubernetes.



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Debugging, local measurements, hardware counters.



SeBS: Cloud Platforms



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“SeBS: a Serverless Benchmark Suite for Function-as-a-Service Computing”, Middleware 2021

 SeBS



Introducing Cloudflare Workers: Run JavaScript Service Workers at the Edge

2017-09-29



APACHE
OpenWhisk

Open-source FaaS, run on any
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Cloudflare

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Local

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 SeBS



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APACHE

Bringing Python to Workers using Pyodide and WebAssembly

2024-04-02



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“SeBS: a Serverless Benchmark Suite for Function-as-a-Service Computing”, Middleware 2021



Introducing Cloudflare Workers: Run JavaScript Service Workers at the Edge

2017-09-29



Bringing Python to Workers using Pyodide and WebAssembly

2024-04-02

Sandboxing AI agents, 100x faster

2026-03-24





FaaS Analysis: Eviction Modeling

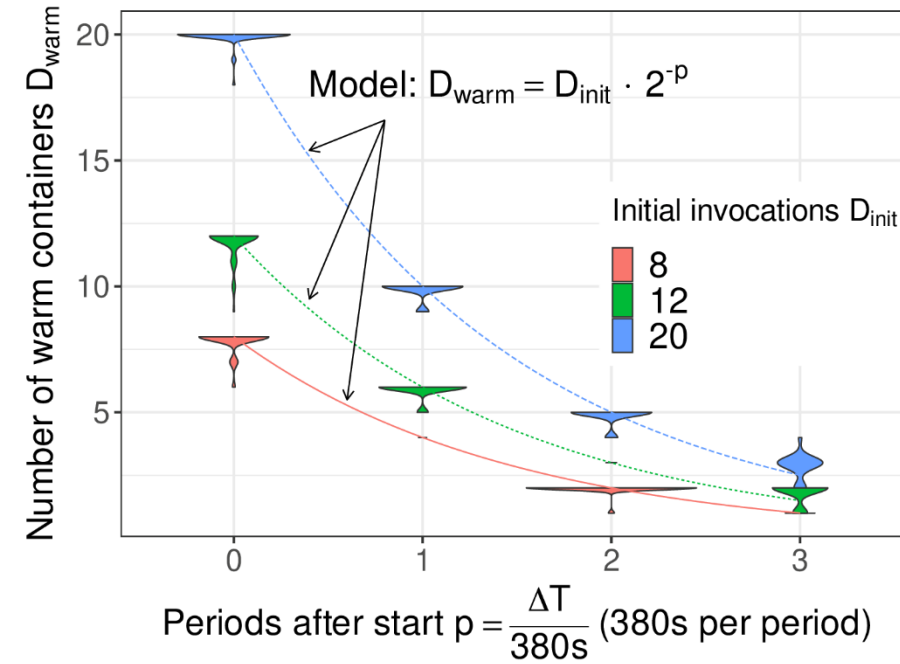
- (1) Which factors impact container eviction?
- (2) Can we recover the original eviction policy?



“SeBS: a Serverless Benchmark Suite for Function-as-a-Service Computing”, Middleware 2021

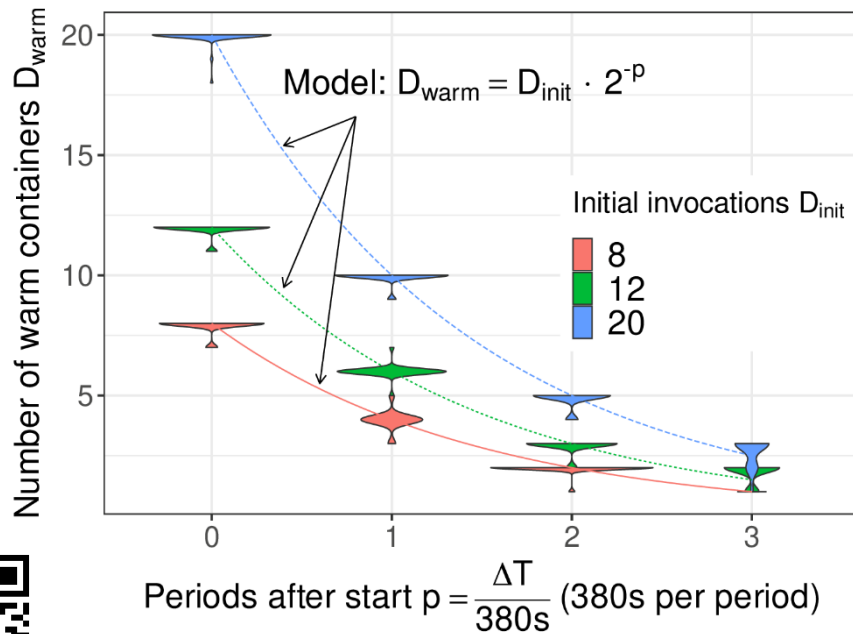
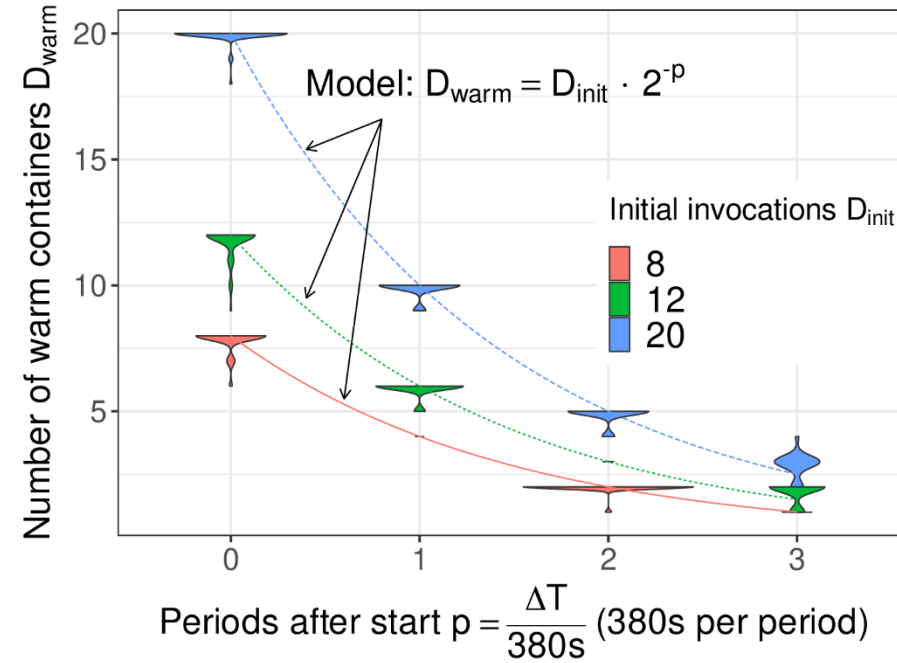
FaaS Analysis: Eviction Modeling

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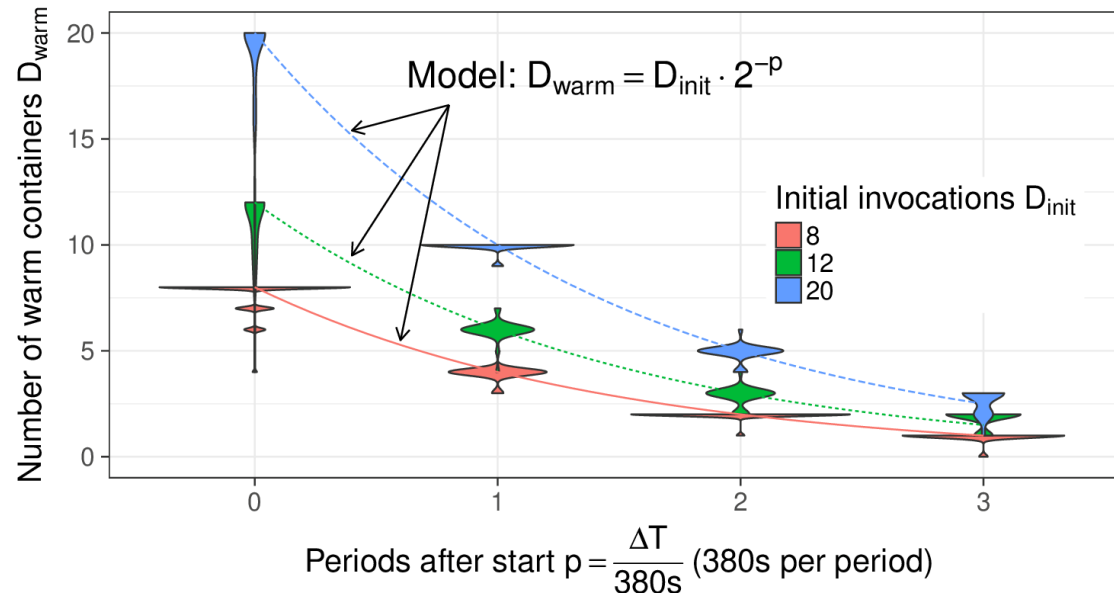
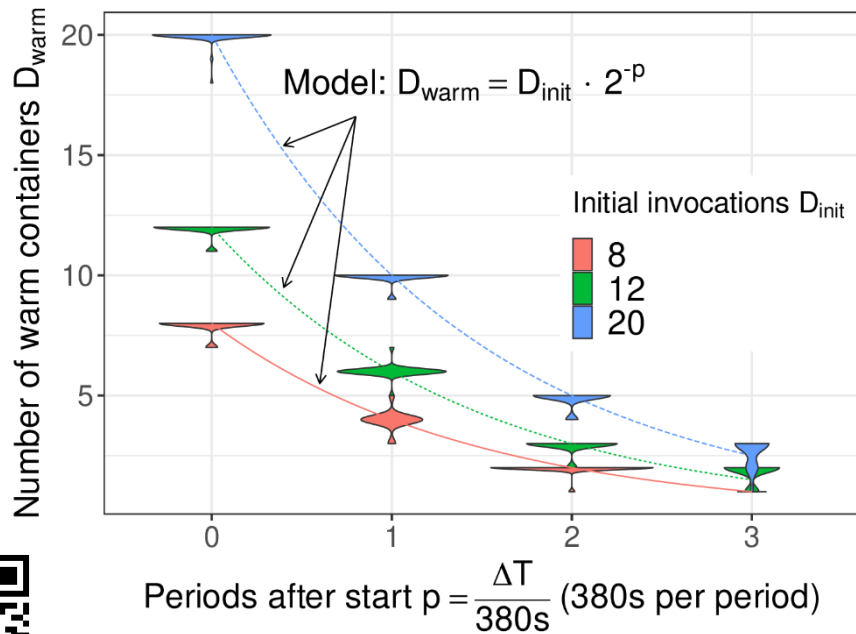
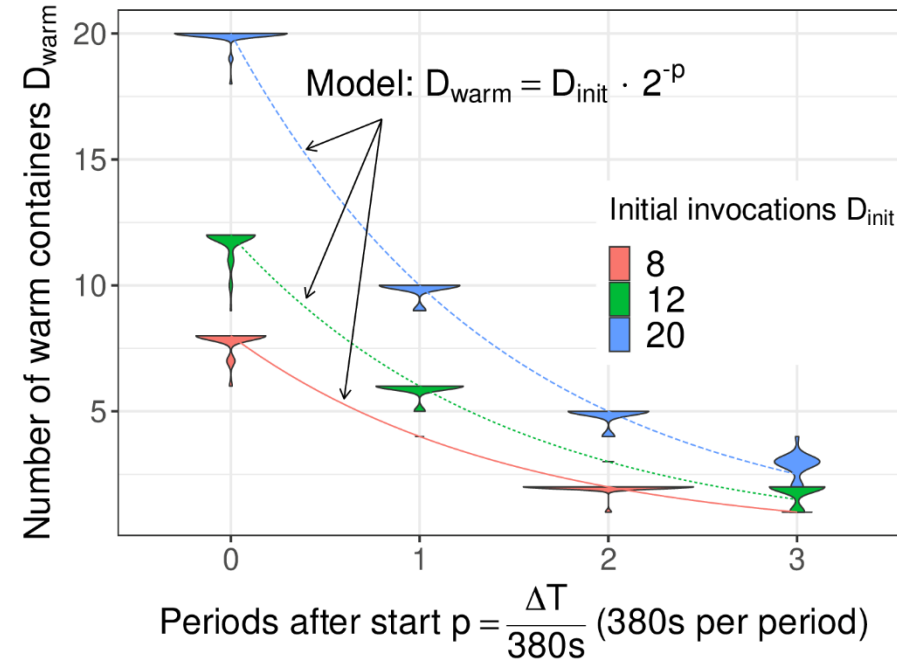
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SeBS-Flow: Let the Work Flow in the Cloud



“SeBS-Flow: Benchmarking Serverless Cloud Function Workflows”, Schmid et al., EuroSys 2025



SeBS-Flow: Let the Work Flow in the Cloud

Azure Durable

```
tasks = []
for i in range(4):
    tasks.append(context.call_activity("process", i))
res = yield context.task_all(parallel_tasks)
```





SeBS-Flow: Let the Work Flow in the Cloud



AWS Step Functions

```

"init": {
  "Type": "Pass",
  "Result": "States.Array(0,
    1, 2, 3)",
  "ResultPath": "$.array",
  "Next": "map"
},
"map": {
  "Type": "Map",
  "ItemsPath": "$.array",
  "Parameters": {
    "payload.$":
      "$$.Map.Item.Value"
  },
  "Iterator": {
    "StartAt": "process",
    "States": {
      "process": {
        "Type": "Task",
        "Resource": "arn:proc",
        "Parameters": {
          "payload.$":
            "$.payload"
        },
        "End": true
      }
    }
  },
  "ResultPath": "$.res",
  "End": true
}

```

Azure Durable 

```

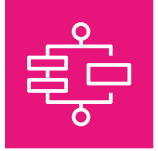
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SeBS-Flow: Let the Work Flow in the Cloud



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Azure Durable 

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res = yield context.task_all(parallel_tasks)

```

```

"assign_array": {
  "assign": [
    {"array": [0, 1, 2, 3]}
  ],
  "process": {
    "call": "exp.exec.map",
    "args": {
      "workflow_id": "map",
      "arguments": "${array}"
    },
    "result": "res"
  }
},
"separate map-workflow":
"main": {
  "params": [ "elem" ],
  "steps": [
    {
      "map": {
        "call": "http.post",
        "args": {
          "url": "google.process",
          "body": {
            "payload": "${elem}"
          }
        },
        "result": "elem"
      }
    },
    { "ret": {
      "return":
        "${elem.body}"
    } }
  ]
}

```





SeBS-Flow: Let the Work Flow in the Cloud



AWS Step Functions

```

"init": {
  "Type": "Pass",
  "Result": "States.Array(0,
    1, 2, 3)",
  "ResultPath": "$.array",
  "Next": "map"
},
"map": {
  "Type": "Map"

```

```

"assign_array": {
  "assign": [
    {"array": [0, 1, 2, 3]}
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    "call": "exp.exec.map",
    "args": {
      "workflow_id": "map",

```

#1 Different Workflow Semantics

#2 Different Workflow Definitions

```

"Parameters": {
  "payload.$":
    "$.payload"
},
"End": true
}
},
"ResultPath": "$.res",
"End": true
}

```

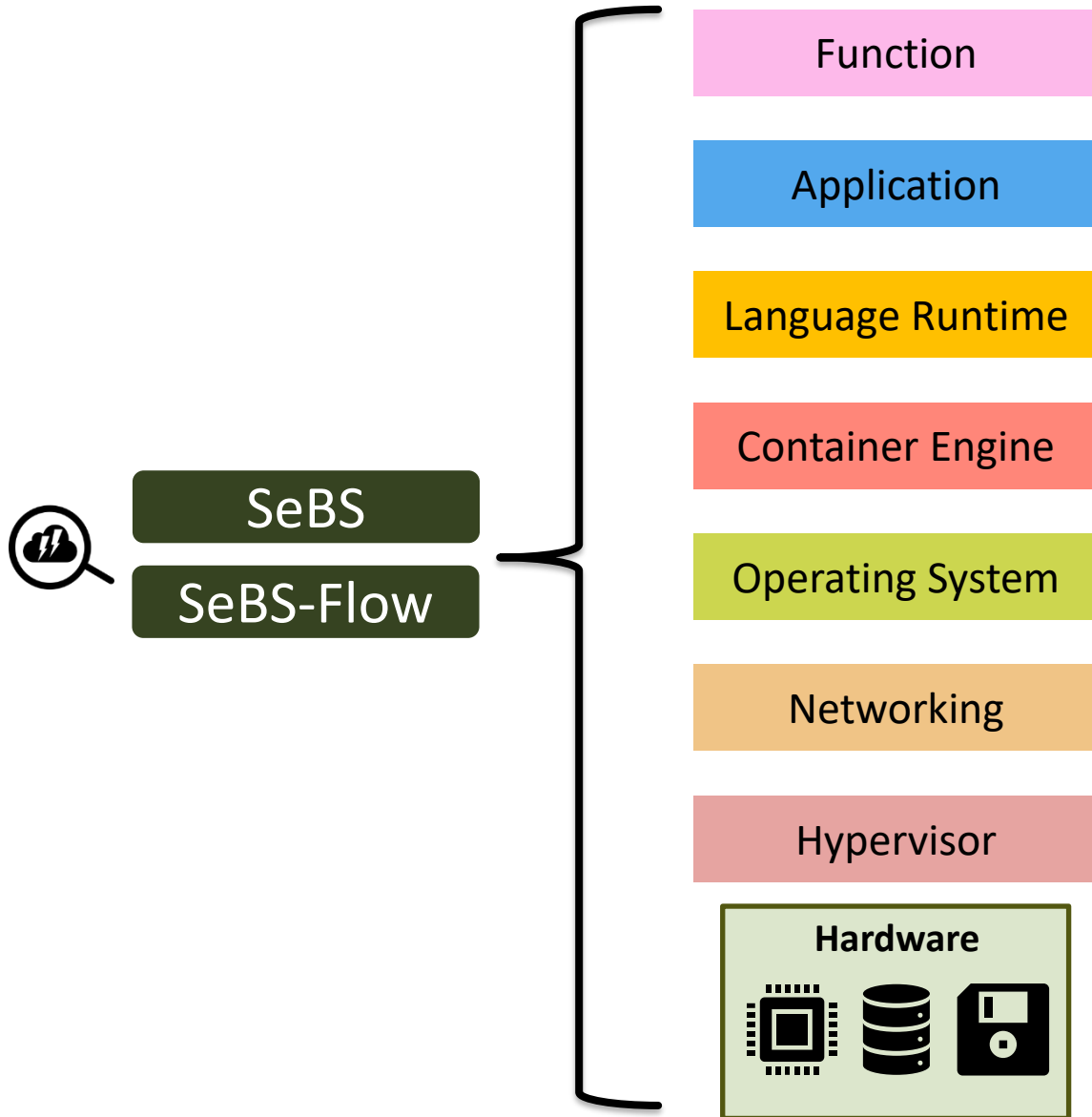
```

"url": "google.process",
"body": {
  "payload": "${elem}"
}
},
"result": "elem" }
},
{ "ret": {
  "return":
    "${elem.body}" } }
] }

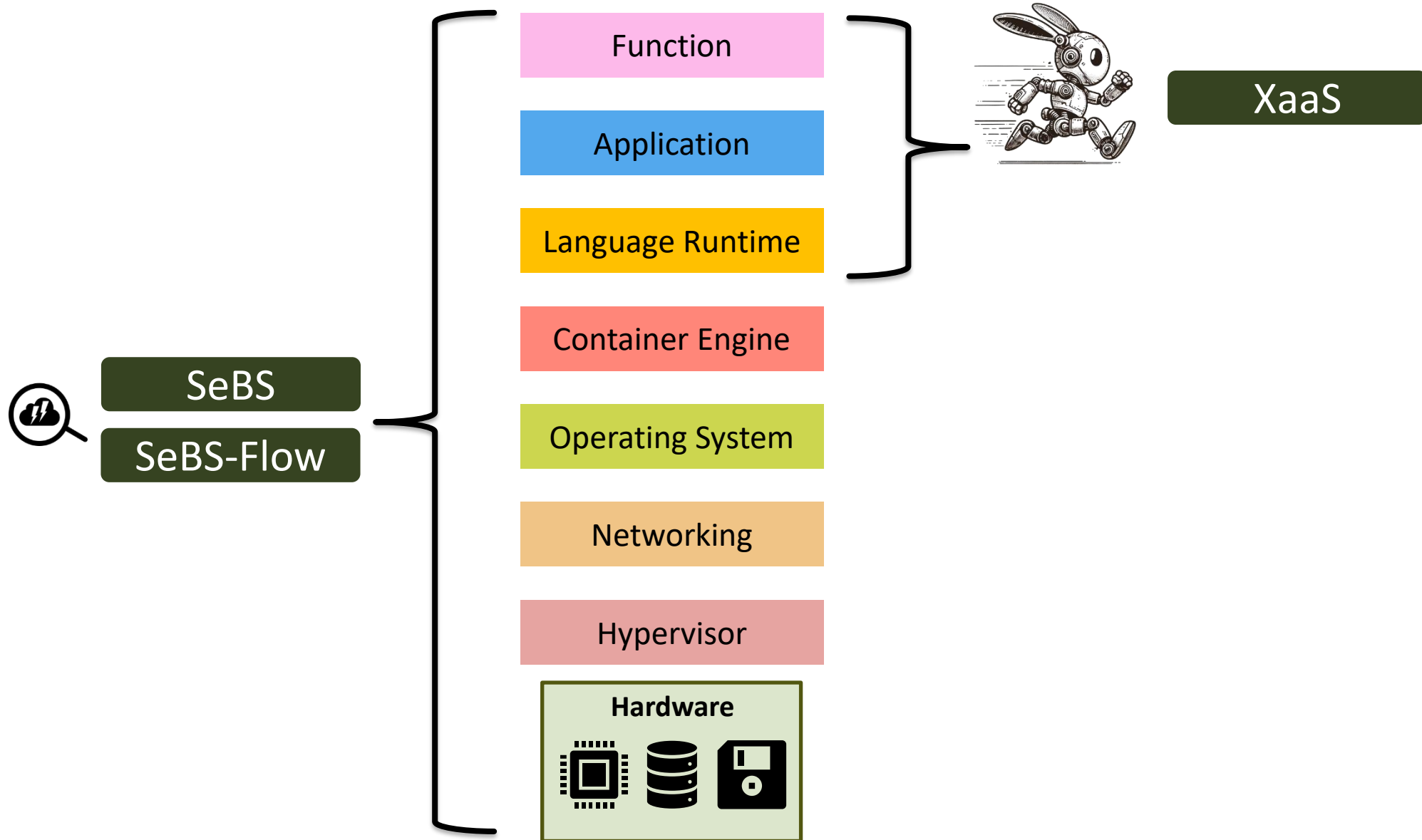
```



AXelerating Serverless Computing: Containerize!



AXelerating Serverless Computing: Containerize!



AXelerating Serverless Computing: Containerize!

XaaS: Acceleration as a Service to Enable Productive High-Performance Cloud Computing

Torsten Hoefler  and Marcin Copik , *ETH Zürich, Zürich, 8093, Switzerland*

Pete Beckman , *Argonne National Laboratory, Lemont, IL, 60439, USA*

Andrew Jones , *Microsoft, Redmond, WA, 98052, USA*

Ian Foster , *Argonne National Laboratory, Lemont, IL, 60439, USA*

Manish Parashar , *Utah University, Salt Lake City, UT, 84112, USA*

Daniel Reed , *Utah University, Salt Lake City, UT, 84117, USA*

Matthias Troyer , *Microsoft, Redmond, WA, 98052, USA*

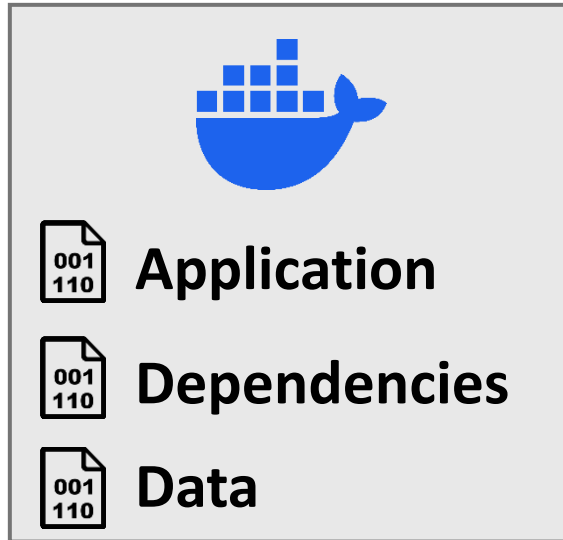
Thomas Schulthess , *Swiss National Supercomputing Centre, Lugano, 6900, Switzerland*

Daniel Ernst , *Nvidia, Santa Clara, CA, 95051, USA*

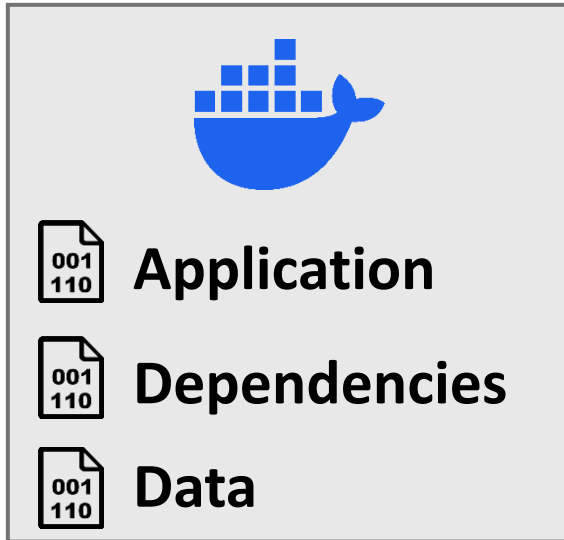
Jack Dongarra , *University of Tennessee, Knoxville, TN, 37996, USA*



Wonderful World of Containers



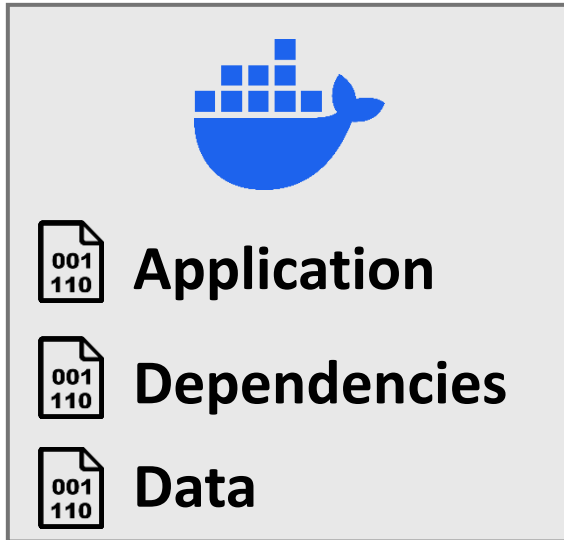
Wonderful World of Containers



docker run gromacs:2025.0

x64 & arm64

Wonderful World of Containers



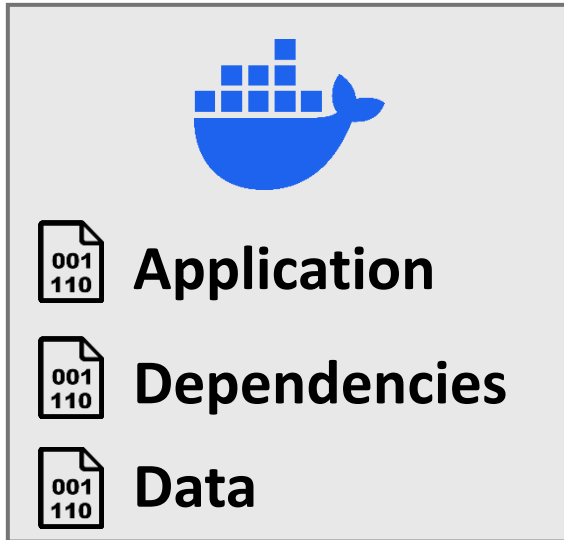
Will it work?



docker run gromacs:2025.0

x64 & arm64

Wonderful World of Containers



Will it work? 

Will it be fast? 

docker run gromacs:2025.0

x64 & arm64

Containers: Portable, but not Performant



gromacs:2025.0, x64 & arm64

Containers: Portable, but not Performant



gromacs:2025.0, x64 & arm64

x86 Execution Time: Intel Xeon Gold 6130

ARM Execution Time: NVIDIA GH200

Execution Time (seconds)

Execution Time (seconds)

Containers: Portable, but not Performant



gromacs:2025.0, x64 & arm64

x86 Execution Time: Intel Xeon Gold 6130

ARM Execution Time: NVIDIA GH200

Execution Time (seconds)

None SSE2 SSE4.1 AVX2_128 AVX_256 AVX_512
 Vectorization Type

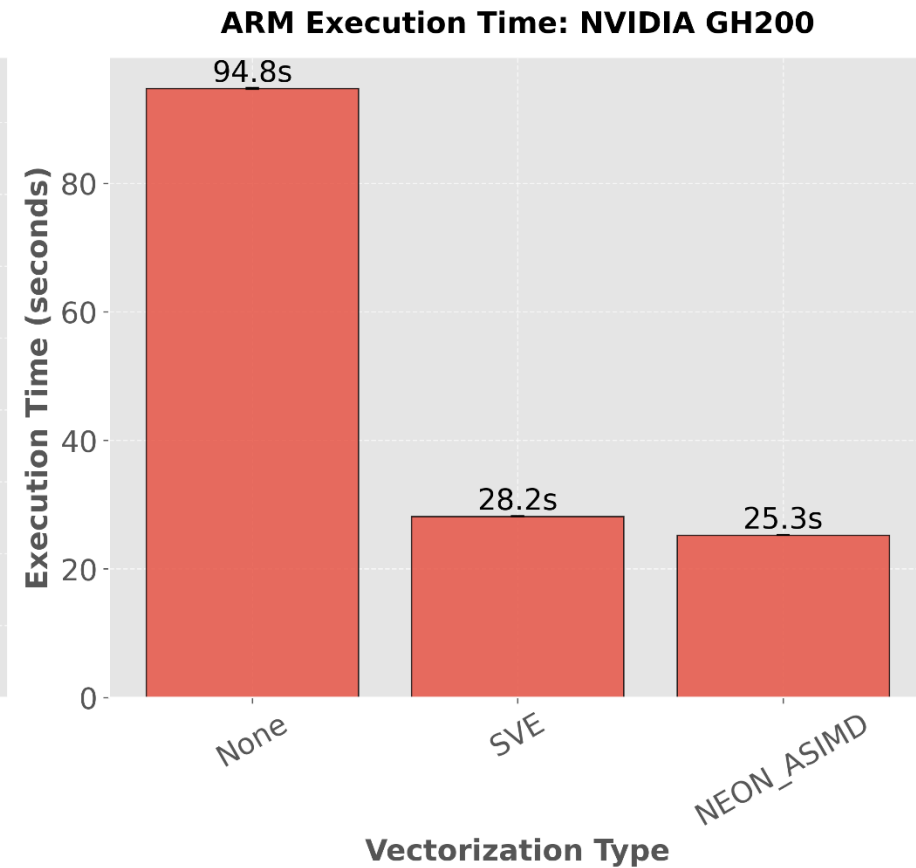
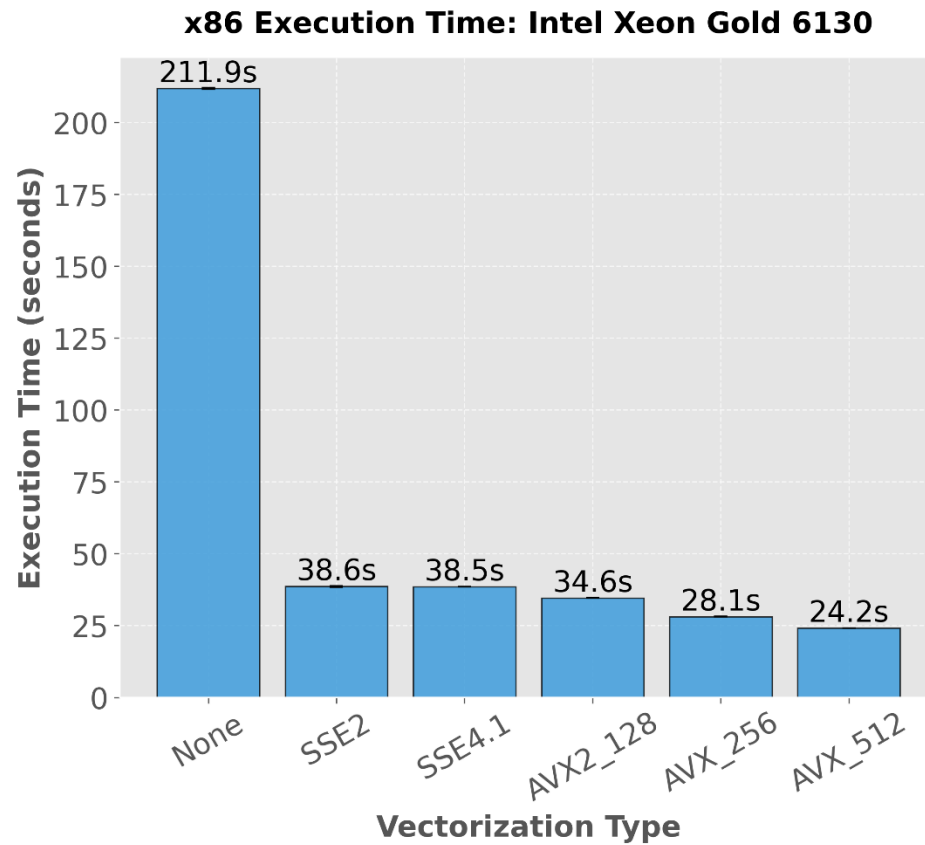
Execution Time (seconds)

None SVE NEON_ASIMD
 Vectorization Type

Containers: Portable, but not Performant



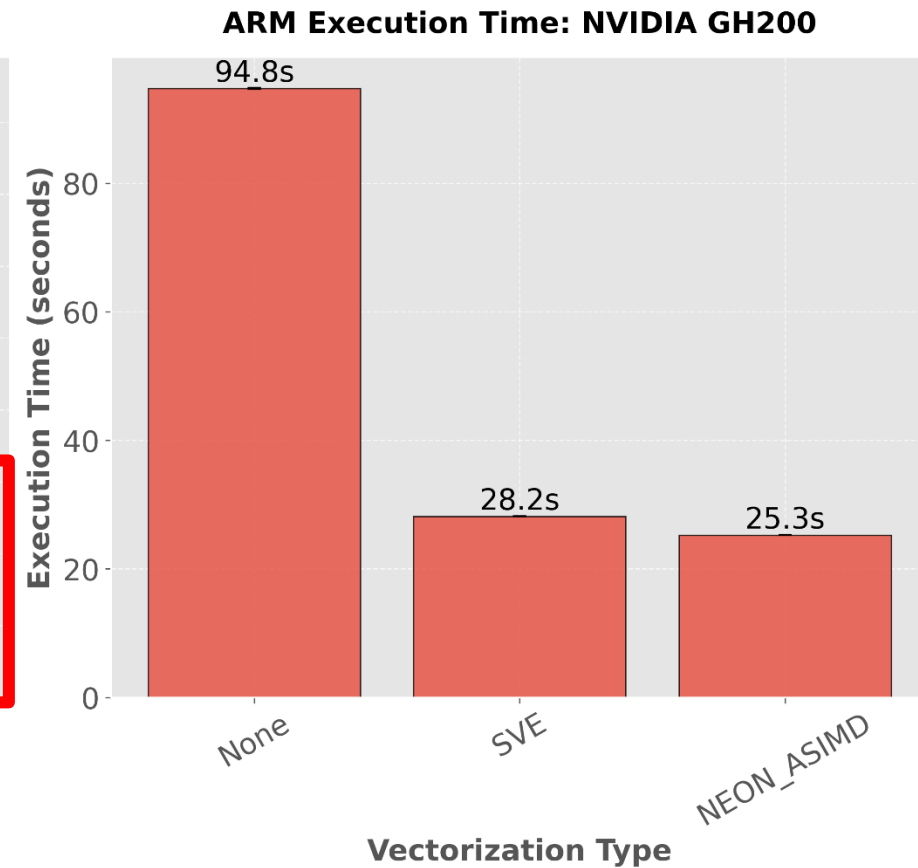
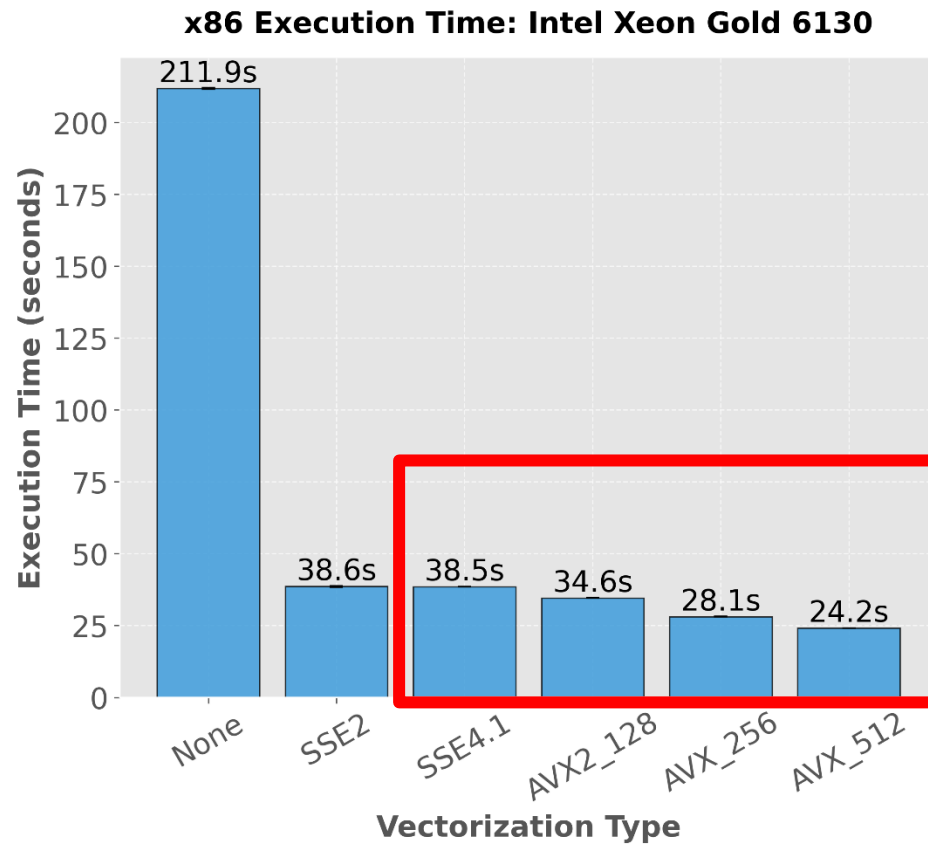
gromacs:2025.0, x64 & arm64



Containers: Portable, but not Performant



gromacs:2025.0, x64 & arm64

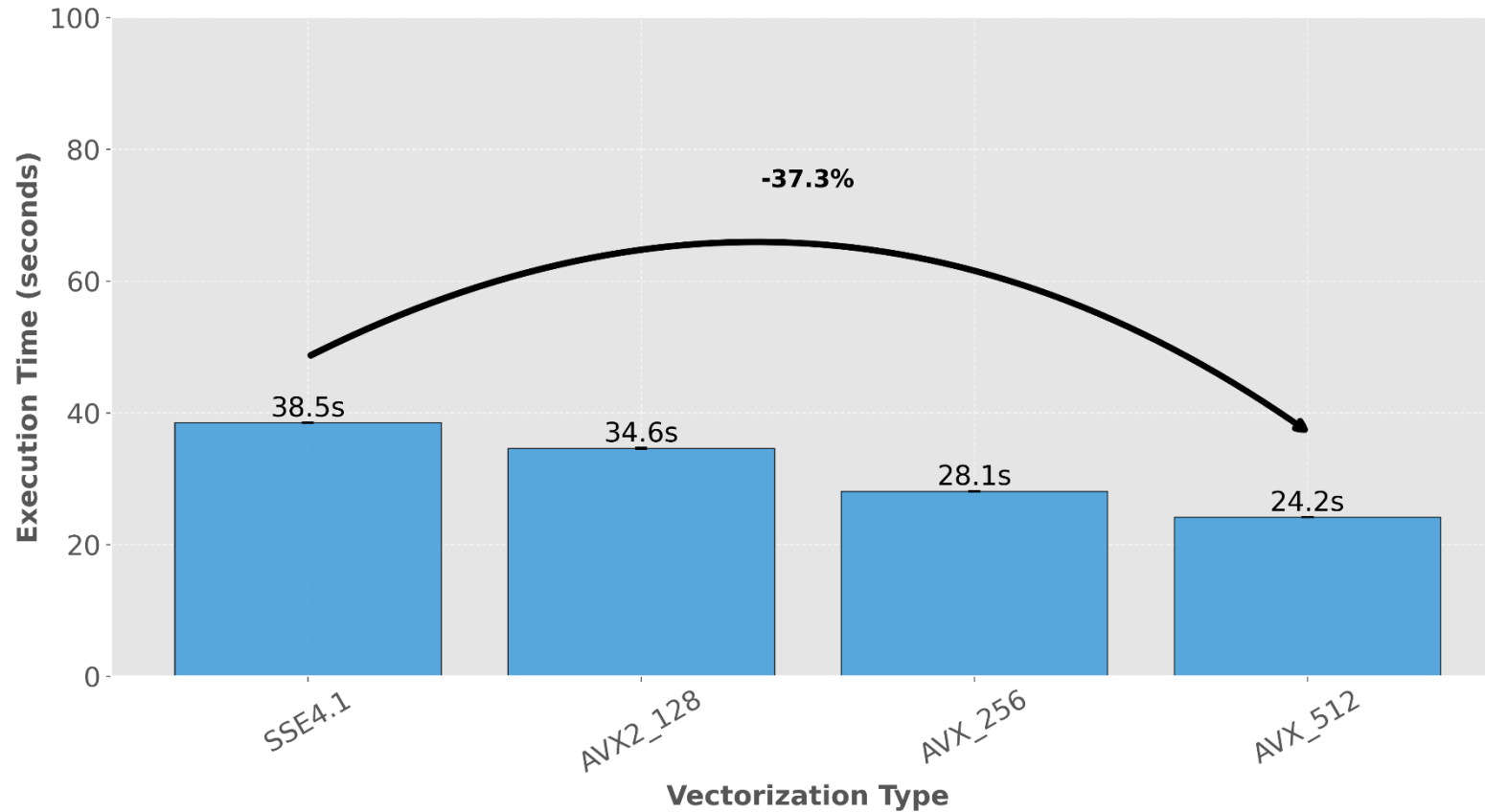


Containers: Portable, but not Performant

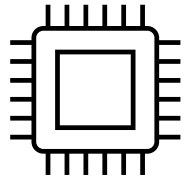


gromacs:2025.0, x64 & arm64

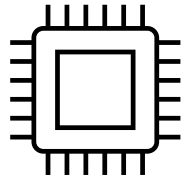
x86 Execution Time: Intel Xeon Gold 6130




Just One More Container...




Just One More Container...



 gromacs:2025.0

sse4.1

 001
110 Dependencies , Data

 gromacs:2025.0

avx-128

 001
110 Dependencies , Data

 gromacs:2025.0

avx-256

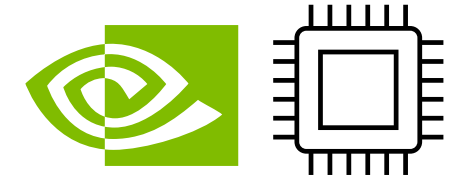
 001
110 Dependencies , Data


 gromacs:2025.0

avx-512


 001
110 Dependencies , Data

Just One More Container...



 gromacs:2025.0

sse4.1

 Dependencies , Data

 gromacs:2025.0

avx-128

 Dependencies , Data

 gromacs:2025.0

avx-256

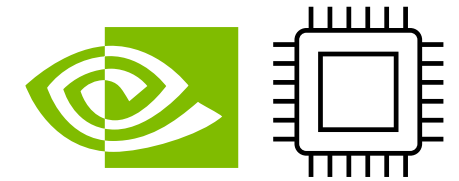
 Dependencies , Data


 gromacs:2025.0

avx-512


 Dependencies , Data

Just One More Container...



 gromacs:2025.0

sse4.1

 001 110 Dependencies , Data

 gromacs:2025.0


avx-128

 001 110 Dependencies , Data


 gromacs:2025.0


avx-256

 001 110 Dependencies , Data


 gromacs:2025.0


avx-512

 001 110 Dependencies , Data


 gromacs:2025.0


sse4.1-cuda

 001 110 Dependencies , Data


 gromacs:2025.0


avx-128-cuda

 001 110 Dependencies , Data


 gromacs:2025.0

avx-256-cuda

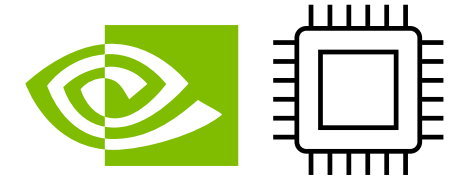
 001 110 Dependencies , Data


 gromacs:2025.0

avx-512-cuda


 001 110 Dependencies , Data

Just One More Container...




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sse4.1

 gromacs:2025.0

avx-128

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 gromacs:2025.0

avx-512


 gromacs:2025.0


sse4.1-cuda

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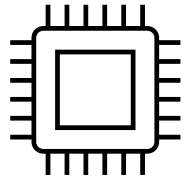
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110 Dependencies , Data


 gromacs:2025.0

avx-512-cuda


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110 Dependencies , Data

Just One More Container...



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sse4.1

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
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 gromacs:2025.0

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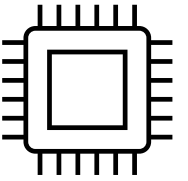
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avx-512-cuda


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avx-128

 gromacs:2025.0


avx-256

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avx-128-cuda

 gromacs:2025.0


avx-256-cuda

 gromacs:2025.0

avx-512-cuda

 gromacs:2025.0

sse4.1-rocm

 gromacs:2025.0

avx-128-rocm

 gromacs:2025.0

avx-256-rocm

 gromacs:2025.0

avx-512-rocm

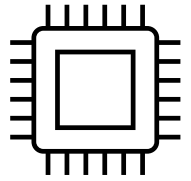
 001
110 Dependencies , Data


 001
110 Dependencies , Data

 001
110 Dependencies , Data


 001
110 Dependencies , Data

Just One More Container...




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sse4.1

 gromacs:2025.0

avx-128

 gromacs:2025.0


avx-256

 gromacs:2025.0


avx-512

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avx-128-cuda

 gromacs:2025.0


avx-256-cuda

 gromacs:2025.0

avx-512-cuda

 gromacs:2025.0


sse4.1-rocm

 001
110 Dependencies , Data


 gromacs:2025.0


avx-128-rocm

 001
110 Dependencies , Data


 gromacs:2025.0

avx-256-rocm

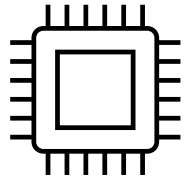
 001
110 Dependencies , Data


 gromacs:2025.0

avx-512-rocm

 001
110 Dependencies , Data

Just One More Container...




 gromacs:2025.0

sse4.1

 gromacs:2025.0

avx-128

 gromacs:2025.0


avx-256

 gromacs:2025.0


avx-512

 gromacs:2025.0


sse4.1-cuda

 gromacs:2025.0

avx-128-cuda

 gromacs:2025.0


avx-256-cuda

 gromacs:2025.0


avx-512-cuda

 gromacs:2025.0


sse4.1-rocm

 gromacs:2025.0

avx-128-rocm

 gromacs:2025.0

avx-256-rocm

 gromacs:2025.0


avx-512-rocm

 gromacs:2025.0


sse4.1-sycl

 gromacs:2025.0

avx-128-sycl

 gromacs:2025.0

avx-256-sycl

 gromacs:2025.0

avx-512-sycl

 001 110 Dependencies , Data

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 001 110 Dependencies , Data

Just One More Container...

Which BLAS library should I use? Which FFT library?

 gromacs:2025.0

sse4.1-cuda

 gromacs:2025.0

sse4.1-rocm

 gromacs:2025.0

sse4.1-sycl

 001 110 Dependencies , Data

 gromacs:2025.0

avx-128-cuda

 gromacs:2025.0

avx-128-rocm

 gromacs:2025.0

avx-128-sycl

 001 110 Dependencies , Data

 gromacs:2025.0

avx-256-cuda

 gromacs:2025.0

avx-256-rocm

 gromacs:2025.0

avx-256-sycl

 001 110 Dependencies , Data

 gromacs:2025.0

avx-512-cuda

 gromacs:2025.0

avx-512-rocm

 gromacs:2025.0

avx-512-sycl

 001 110 Dependencies , Data



Just One More Container...

Which BLAS library should I use? Which FFT library?

 gromacs:2025.0

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 gromacs:2025.0

Should we use OpenMP? Which MPI?

 gromacs:2025.0

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 gromacs:2025.0

 gromacs:2025.0

sse4.1-rocm

avx-128-rocm

avx-256-rocm

avx-512-rocm

 gromacs:2025.0

 gromacs:2025.0

 gromacs:2025.0

 gromacs:2025.0

sse4.1-sycl

avx-128-sycl

avx-256-sycl

avx-512-sycl

 001 110 Dependencies , Data

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 gromacs:2025.0

sse4.1-rocm

avx-128-rocm

avx-256-rocm

avx-512-rocm

What if container has CUDA 12.9, and my system driver is at 12.1?
For which CUDA architecture should we emit code?

001
110 Dependencies , Data

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110 Dependencies , Data

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110 Dependencies , Data

001
110 Dependencies , Data

HPC Specialization Points

HPC Specialization Points

Vectorization

Acceleration

Parallelism & Network Communication

Performance Libraries

System-Specific Optimizations

HPC Specialization Points

Vectorization

Acceleration

Parallelism & Network Communication

Performance Libraries

System-Specific Optimizations

Specialization Points

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Specialization Points

Difficult to build one binary that supports
all possible options!

HPC Specialization Points

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WheelNext

HPC Specialization Points

Vectorization

Acceleration

Parallelism & Network Communication

Performance Libraries

System-Specific Optimizations

Specialization Points

Difficult to build one binary that supports all possible options!



WheelNext

blas-lapack-variant-provider

This is a plugin for the proposed [wheel variants implementation](#) that provides BLAS/LAPACK library selection.

This plugin always returns a fixed list of supported variants, and so can be used as a build-time plugin.

HPC Specialization Points

Vectorization

Acceleration

Parallelism & Network Communication

Performance Libraries

System-Specific Optimizations

Specialization Points

Difficult to build one binary that supports all possible options!



WheelNext

blas-lapack-variant-provider

This is a plugin for the proposed [wheel variants implementation](#) that provides BLAS/LAPACK library selection.

This plugin always returns a fixed list of supported variants, and so can be used as a build-time plugin.

HPC is not only Python!
We need a **general-purpose** solution.

How to Provide Portability for HPC Software?

How to Provide Portability for HPC Software?



**Building
Source**

How to Provide Portability for HPC Software?



**Building
Source**



**Relinking
Dependencies**

How to Provide Portability for HPC Software?



**Building
Source**

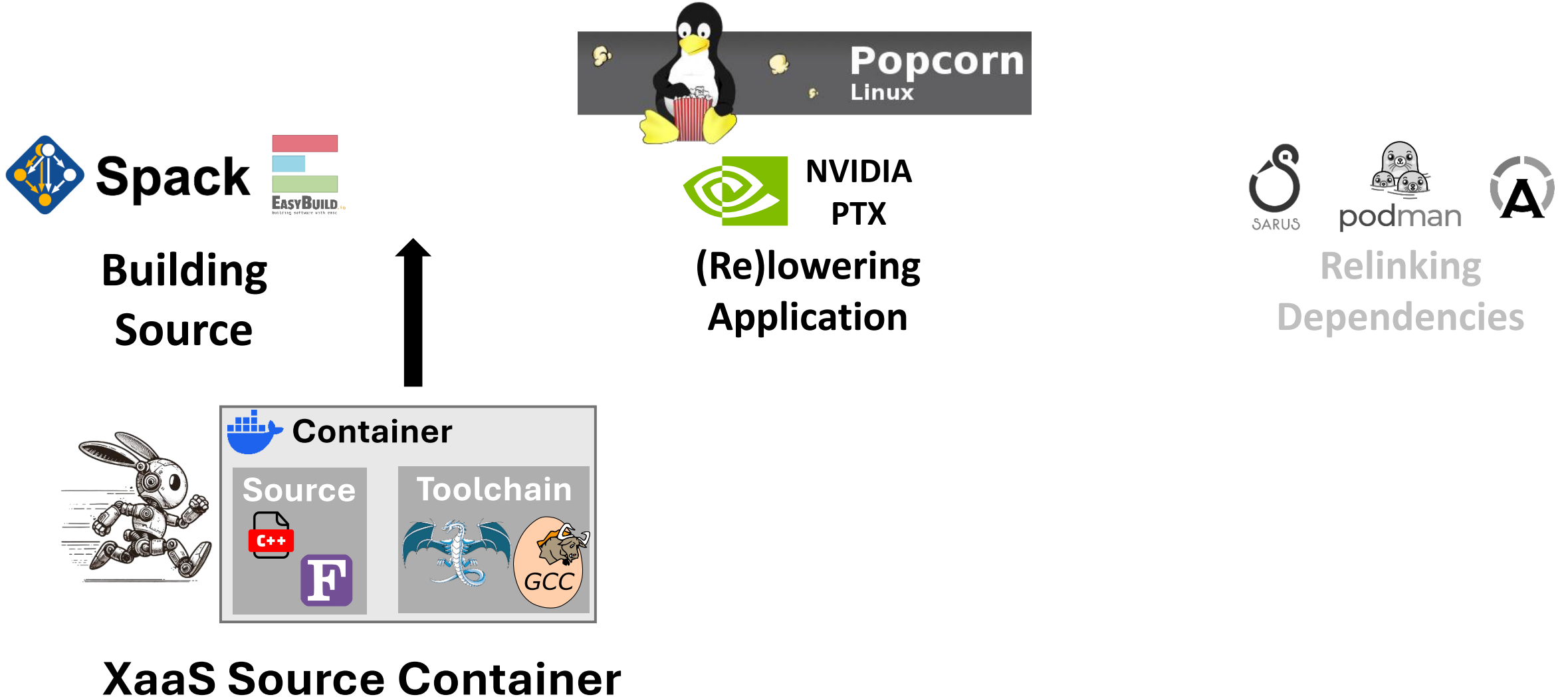


**(Re)lowering
Application**

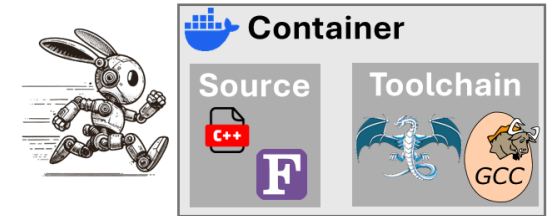


**Relinking
Dependencies**

How to Provide Portability for HPC Software?



Configuring Containers for HPC Specializations



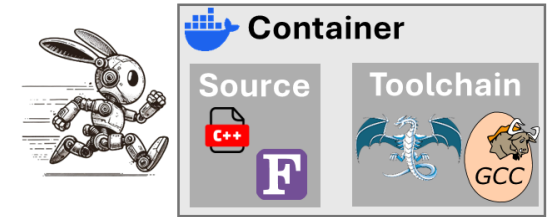
XaaS Source Container

```
{
  "gpu_build": {"value": true, "build_flag": "-DGMX_GPU"},
  "gpu_backends": {
    "CUDA": {"min_version": "12.1", "flag": "-DGMX_GPU=CUDA"},
    "HIP": {"min_version": "5.4.3", "flag": "-DGMX_GPU=HIP"}
  },
  "vectorization": {
    "None": {"flag": "-DGMX_SIMD=None"},
    "SSE4.1": {"flag": "-DGMX_SIMD=SSE4.1"},
    "AVX2_256": {"flag": "-DGMX_SIMD=AVX2_256"},
    "AVX_512": {"flag": "-DGMX_SIMD=AVX_512"},
    "ARM_NEON_ASIMD": {"flag": "-DGMX_SIMD=ARM_NEON_ASIMD"}
  }
}
```



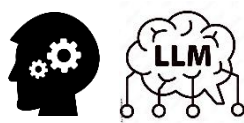
Specialization Discovery

Configuring Containers for HPC Specializations





XaaS Source Container

```
{
  "gpu_build": {"value": true, "build_flag": "-DGMX_GPU"},
  "gpu_backends": {
    "CUDA": {"min_version": "12.1", "flag": "-DGMX_GPU=CUDA"},
    "HIP": {"min_version": "5.4.3", "flag": "-DGMX_GPU=HIP"}
  },
  "vectorization": {
    "None": {"flag": "-DGMX_SIMD=None"},
    "SSE4.1": {"flag": "-DGMX_SIMD=SSE4.1"},
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    "AVX_512": {"flag": "-DGMX_SIMD=AVX_512"},
    "ARM_NEON_ASIMD": {"flag": "-DGMX_SIMD=ARM_NEON_ASIMD"}
  }
}
```



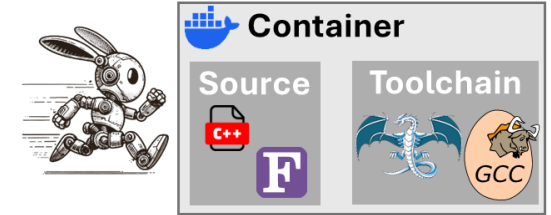
Specialization Discovery

GROMACS
In-Context Learning
 **Gemini 1.5 & 2.0**
F1 Scores: 0.86 – 0.99

llama.cpp
Generalization
 **GPT-o3**
F1 Scores: 0.73 - 0.79

F1 Score: harmonic mean between **precision** (minimize false positives) and **recall** (minimize false negatives).

Configuring Containers for HPC Specializations



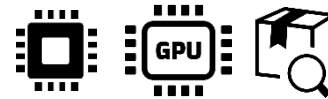
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  "gpu_build": {"value": true, "build_flag": "-DGMX_GPU"},
  "gpu_backends": {
    "CUDA": {"min_version": "12.1", "flag": "-DGMX_GPU=CUDA"},
    "HIP": {"min_version": "5.4.3", "flag": "-DGMX_GPU=HIP"}
  },
  "vectorization": {
    "None": {"flag": "-DGMX_SIMD=None"},
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    "AVX_512": {"flag": "-DGMX_SIMD=AVX_512"},
    "ARM_NEON_ASIMD": {"flag": "-DGMX_SIMD=ARM_NEON_ASIMD"}
  }
}
```

```
{
  "CPU Info": {
    "Architecture": "x86_64",
    "Vectorization": [
      "avx512f", "avx", "avx2", "sse4_1"
    ]
  },
  "GPU Backends": {
    "CUDA": { "version": "12.1",
      "lib": ["/lib/libcuda.so.1"],
    }
  }
}
```

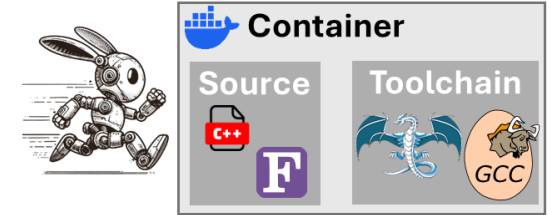


Specialization Discovery



System Discovery

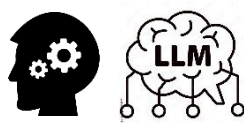
Configuring Containers for HPC Specializations



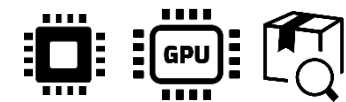
XaaS Source Container

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{
  "gpu_build": {"value": true, "build_flag": "-DGMX_GPU"},
  "gpu_backends": {
    "CUDA": {"min_version": "12.1", "flag": "-DGMX_GPU=CUDA"},
    "HIP": {"min_version": "5.4.3", "flag": "-DGMX_GPU=HIP"}
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    "ARM_NEON_ASIMD": {"flag": "-DGMX_SIMD=ARM_NEON_ASIMD"}
  }
}
```

```
{
  "CPU Info": {
    "Architecture": "x86_64",
    "Vectorization": [
      "avx512f", "avx", "avx2", "sse4_1"
    ]
  },
  "GPU Backends": {
    "CUDA": { "version": "12.1",
      "lib": ["/lib/libcuda.so.1"],
    }
  }
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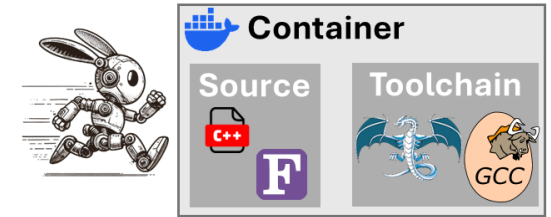


Specialization Discovery



System Discovery

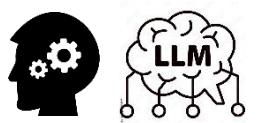
Configuring Containers for HPC Specializations



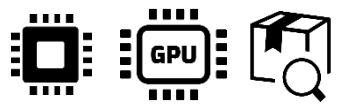
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    "AVX_512": {"flag": "-DGMX_SIMD=AVX_512"},
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  }
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    "Architecture": "x86_64",
    "Vectorization": [
      "avx512f", "avx", "avx2", "sse4_1"
    ]
  },
  "GPU Backends": {
    "CUDA": { "version": "12.1",
      "lib": ["/lib/libcuda.so.1"],
    }
  }
}
```



Specialization Discovery



System Discovery

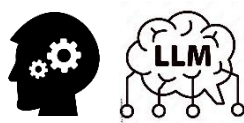
Configuring Containers for HPC Specializations



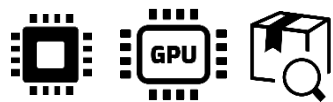
XaaS Source Container

```
{
  "gpu_build": {"value": true, "build_flag": "-DGMX_GPU"},
  "gpu_backends": {
    "CUDA": {"min_version": "12.1", "flag": "-DGMX_GPU=CUDA"},
    "HIP": {"min_version": "5.4.3", "flag": "-DGMX_GPU=HIP"}
  },
  "vectorization": {
    "None": {"flag": "-DGMX_SIMD=None"},
    "SSE4.1": {"flag": "-DGMX_SIMD=SSE4.1"},
    "AVX2_256": {"flag": "-DGMX_SIMD=AVX2_256"},
    "AVX_512": {"flag": "-DGMX_SIMD=AVX_512"},
    "ARM_NEON_ASIMD": {"flag": "-DGMX_SIMD=ARM_NEON_ASIMD"}
  }
}
```

```
{
  "CPU Info": {
    "Architecture": "x86_64",
    "Vectorization": [
      "avx512f", "avx", "avx2", "sse4_1"
    ]
  },
  "GPU Backends": {
    "CUDA": { "version": "12.1",
      "lib": ["/lib/libcuda.so.1"],
    }
  }
}
```

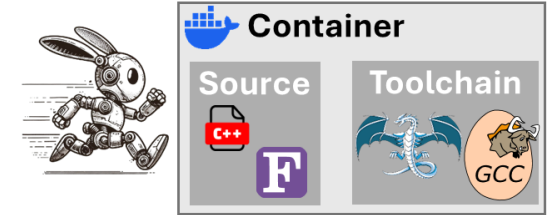


Specialization Discovery



System Discovery

Configuring Containers for HPC Specializations

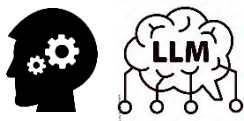


XaaS Source Container

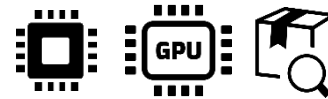
```
{
  "gpu_build": {"value": true, "build_flag": "-DGMX_GPU"},
  "gpu_backends": {
    "CUDA": {"min_version": "12.1", "flag": "-DGMX_GPU=CUDA"},
    "HIP": {"min_version": "5.4.3", "flag": "-DGMX_GPU=HIP"}
  },
  "vectorization": {
    "None": {"flag": "-DGMX_SIMD=None"},
    "SSE4.1": {"flag": "-DGMX_SIMD=SSE4.1"},
    "AVX2_256": {"flag": "-DGMX_SIMD=AVX2_256"},
    "AVX_512": {"flag": "-DGMX_SIMD=AVX_512"},
    "ARM_NEON_ASIMD": {"flag": "-DGMX_SIMD=ARM_NEON_ASIMD"}
  }
}
```

```
{
  "CPU Info": {
    "Architecture": "x86_64",
    "Vectorization": [
      "avx512f", "avx", "avx2", "sse4_1"
    ]
  },
  "GPU Backends": {
    "CUDA": { "version": "12.1",
      "lib": ["/lib/libcuda.so.1"],
    }
  }
}
```

```
"vectorization_flags": {
  "SSE4.1": "-DGMX_SIMD=SSE4.1",
  "AVX_512": "-DGMX_SIMD=AVX_512",
  "AVX2_256": "-DGMX_SIMD=AVX2_256"
},
```

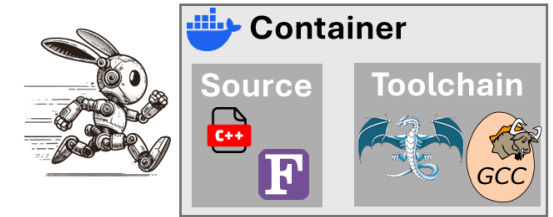


Specialization Discovery



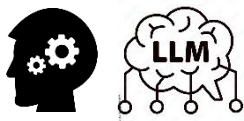
System Discovery

Configuring Containers for HPC Specializations



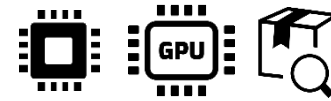
XaaS Source Container

```
{
  "gpu_build": {"value": true, "build_flag": "-DGMX_GPU"},
  "gpu_backends": {
    "CUDA": {"min_version": "12.1", "flag": "-DGMX_GPU=CUDA"},
    "HIP": {"min_version": "5.4.3", "flag": "-DGMX_GPU=HIP"}
  },
  "vectorization": {
    "None": {"flag": "-DGMX_SIMD=None"},
    "SSE4.1": {"flag": "-DGMX_SIMD=SSE4.1"},
    "AVX2_256": {"flag": "-DGMX_SIMD=AVX2_256"},
    "AVX_512": {"flag": "-DGMX_SIMD=AVX_512"},
    "ARM_NEON_ASIMD": {"flag": "-DGMX_SIMD=ARM_NEON_ASIMD"}
  }
}
```



Specialization Discovery

```
{
  "CPU Info": {
    "Architecture": "x86_64",
    "Vectorization": [
      "avx512f", "avx", "avx2", "sse4_1"
    ]
  },
  "GPU Backends": {
    "CUDA": { "version": "12.1",
      "lib": ["/lib/libcuda.so.1"],
    }
  }
}
```



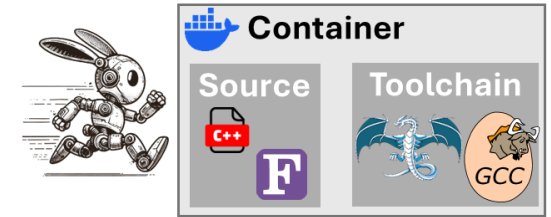
System Discovery

```
{
  "common_specialization": {
    "vectorization_flags": {
      "SSE4.1": "-DGMX_SIMD=SSE4.1",
      "AVX_512": "-DGMX_SIMD=AVX_512",
      "AVX2_256": "-DGMX_SIMD=AVX2_256"
    },
    "gpu_backends": {
      "CUDA": { "version": "12.1",
        "flag": "-DGMX_GPU=CUDA",
      },
    }
  }
}
```



Feature Intersection

XaaS Source Containers Deployment

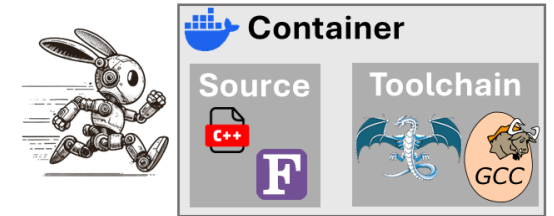


XaaS Source Container

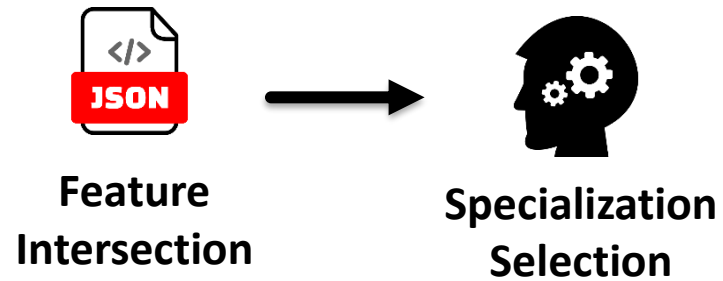


**Feature
Intersection**

XaaS Source Containers Deployment



XaaS Source Container

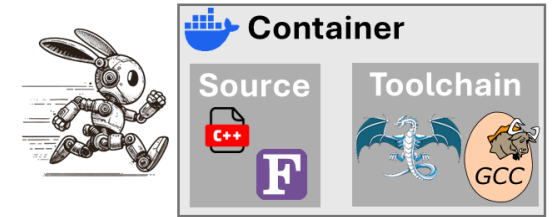


Vectorization: AVX-512

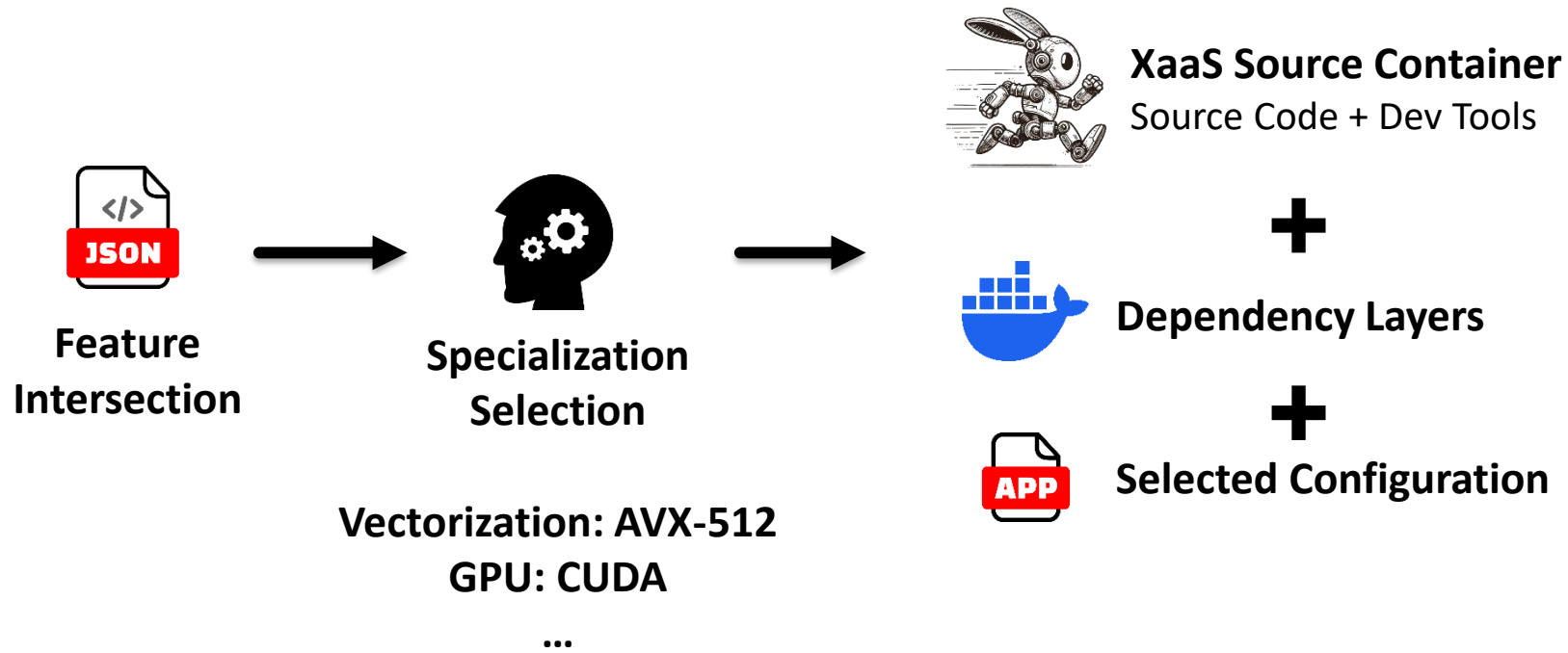
GPU: CUDA

...

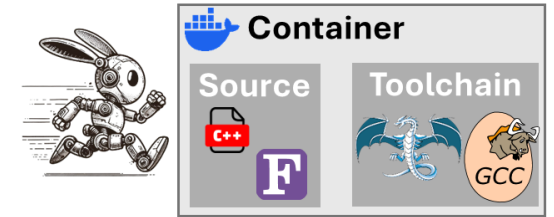
XaaS Source Containers Deployment



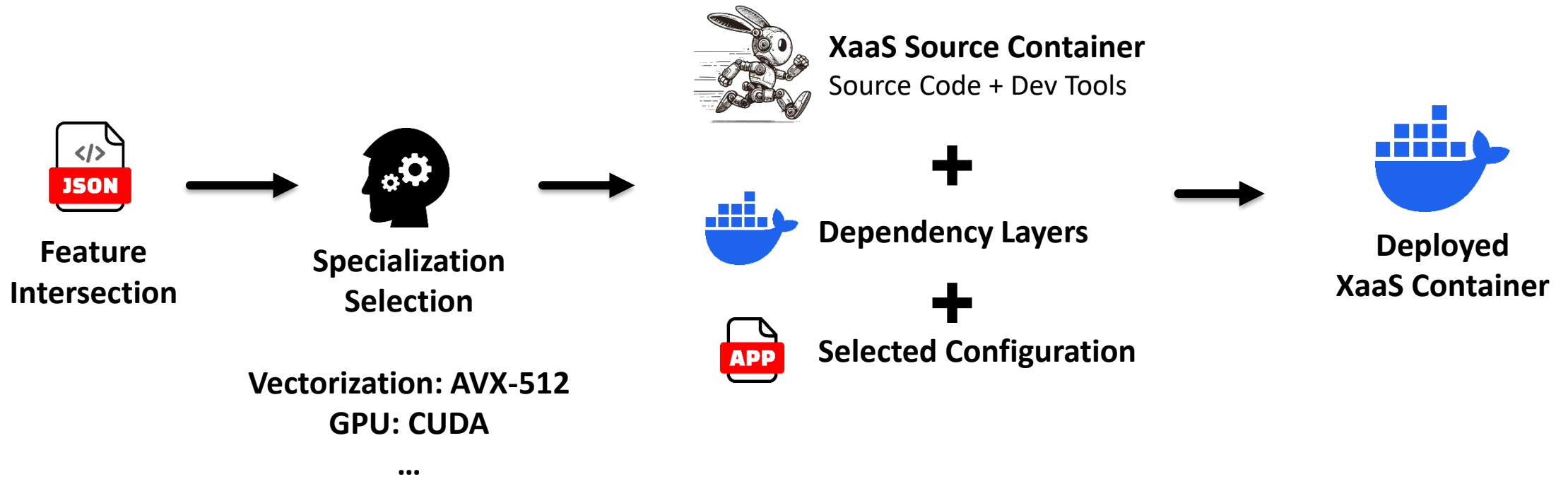
XaaS Source Container



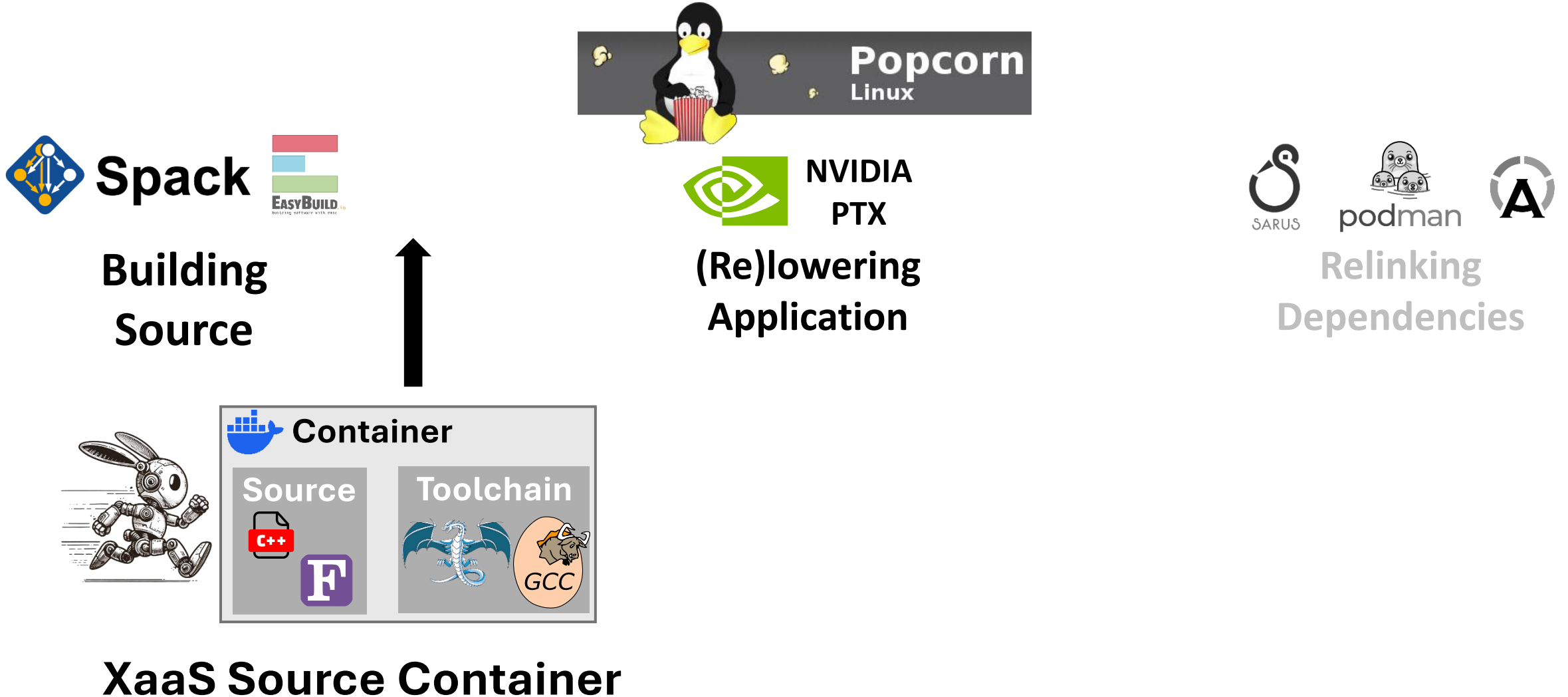
XaaS Source Containers Deployment



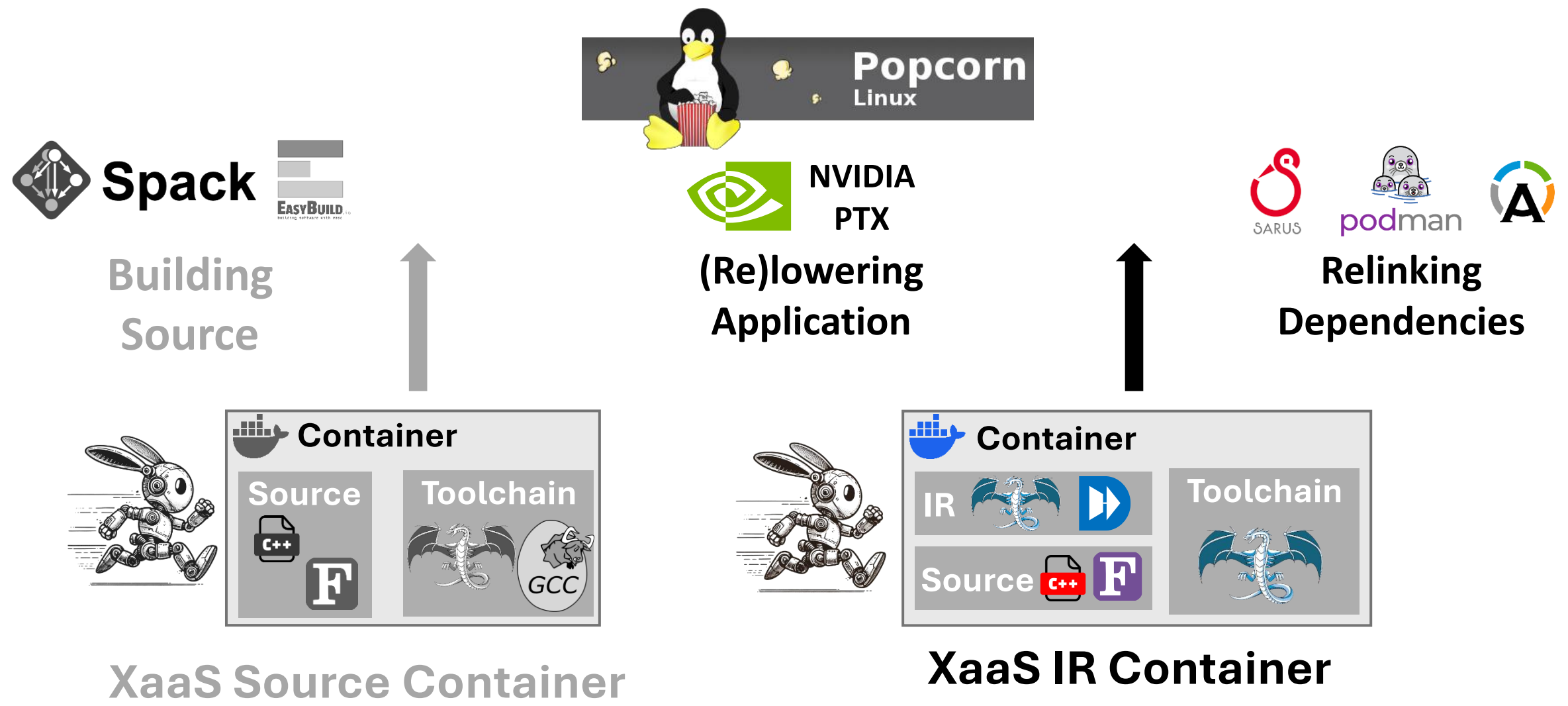
XaaS Source Container



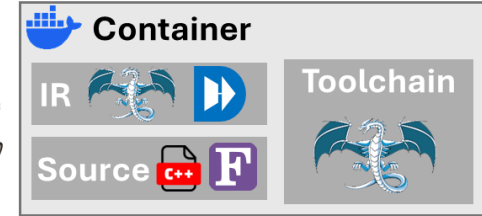
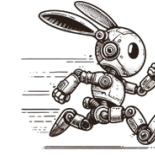
How to Provide Portability for HPC Software?



How to Provide Portability for HPC Software?

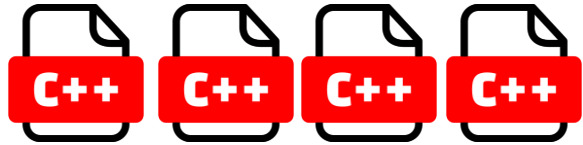


XaaS IR Containers: Eliminating Redundancy



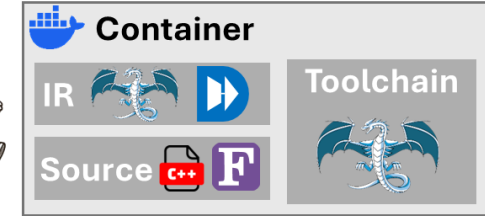
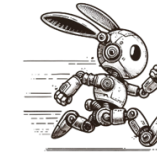
XaaS IR Container

XaaS IR Containers: Eliminating Redundancy



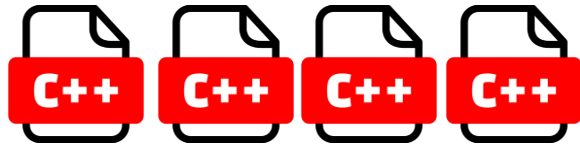
Config N° 1

AVX-256, no GPU, OpenMP



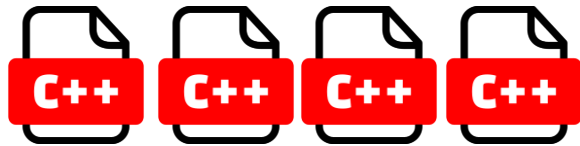
XaaS IR Container

XaaS IR Containers: Eliminating Redundancy



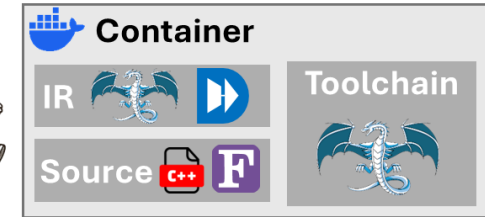
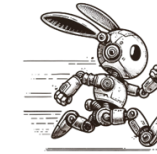
Config N° 1

AVX-256, no GPU, OpenMP



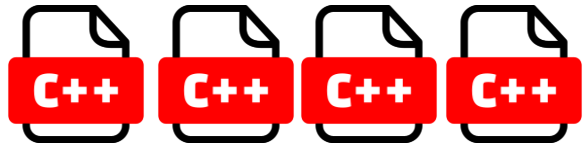
Config N° 2

AVX-512, CUDA, MPI

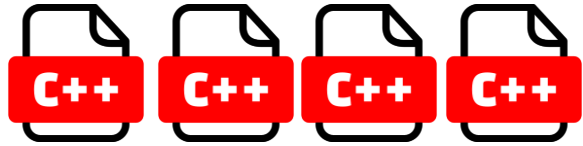


XaaS IR Container

XaaS IR Containers: Eliminating Redundancy



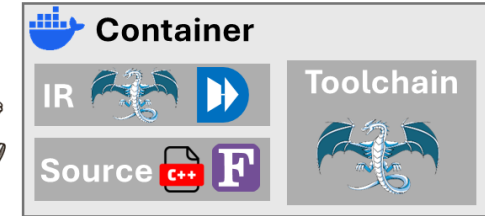
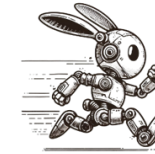
Config N° 1
AVX-256, no GPU, OpenMP



Config N° 2
AVX-512, CUDA, MPI

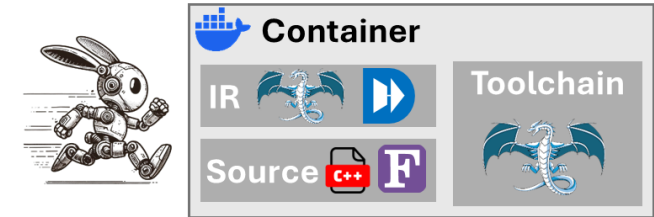


Config N° 3
AVX-256, CUDA, MPI

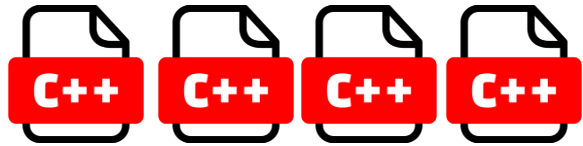


XaaS IR Container

XaaS IR Containers: Eliminating Redundancy



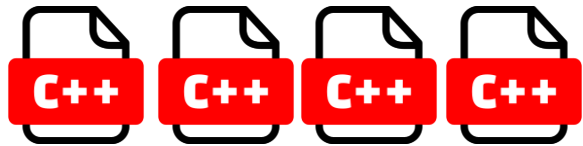
XaaS IR Container



Config N° 1

AVX-256, no GPU, OpenMP

✗ Compile-time definitions.



Config N° 2

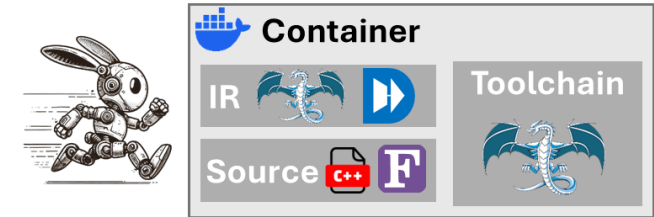
AVX-512, CUDA, MPI



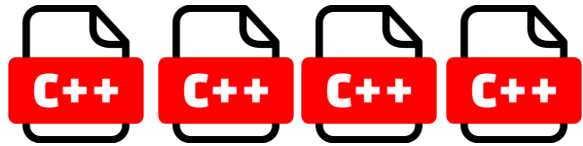
Config N° 3

AVX-256, CUDA, MPI

XaaS IR Containers: Eliminating Redundancy



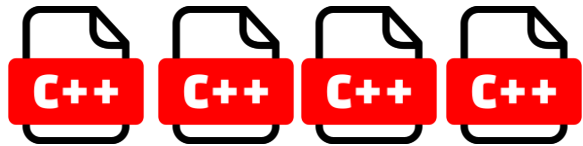
XaaS IR Container



Config N° 1

AVX-256, no GPU, OpenMP

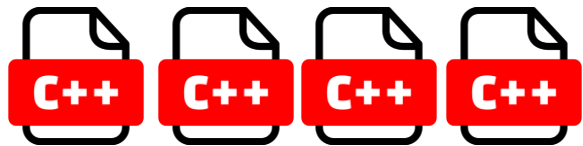
✗ Compile-time definitions.



Config N° 2

AVX-512, CUDA, MPI

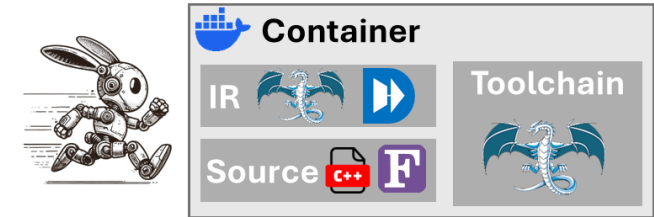
✗ Include paths in build directories.



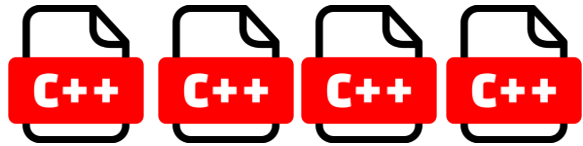
Config N° 3

AVX-256, CUDA, MPI

XaaS IR Containers: Eliminating Redundancy

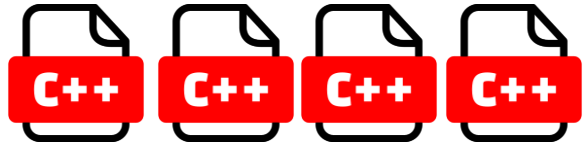


XaaS IR Container



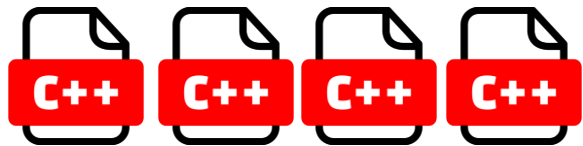
Config N° 1

AVX-256, no GPU, OpenMP



Config N° 2

AVX-512, CUDA, MPI

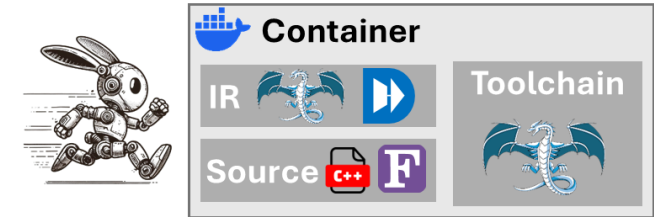


Config N° 3

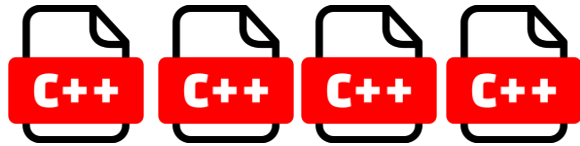
AVX-256, CUDA, MPI

- ✗ Compile-time definitions.
- ✗ Include paths in build directories.
- ✗ Vectorization and architecture flags.

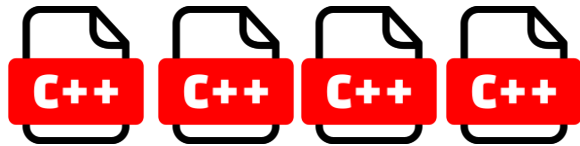
XaaS IR Containers: Eliminating Redundancy



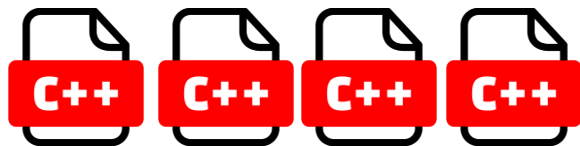
XaaS IR Container



Config N° 1
AVX-256, no GPU, OpenMP



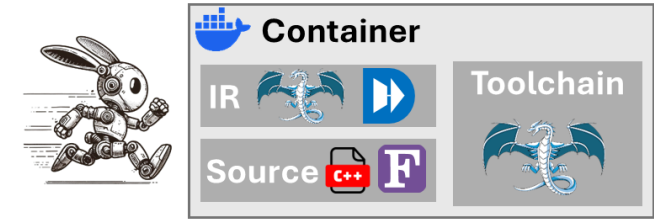
Config N° 2
AVX-512, CUDA, MPI



Config N° 3
AVX-256, CUDA, MPI

- ✗ Compile-time definitions.
- ✗ Include paths in build directories.
- ✗ Vectorization and architecture flags.
- ✗ OpenMP flags.

XaaS IR Containers: Eliminating Redundancy



XaaS IR Container



Config N° 1

AVX-256, no GPU, OpenMP



Config N° 2

AVX-512, CUDA, MPI

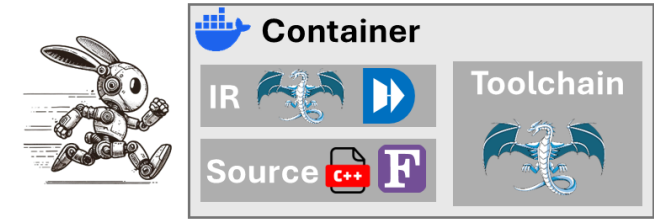


Config N° 3

AVX-256, CUDA, MPI

- ✗ Compile-time definitions.
- ✗ Include paths in build directories.
- ✗ Vectorization and architecture flags.
- ✗ OpenMP flags.

XaaS IR Containers: Eliminating Redundancy



XaaS IR Container



Config N° 1

AVX-256, no GPU, OpenMP

Config N° 2

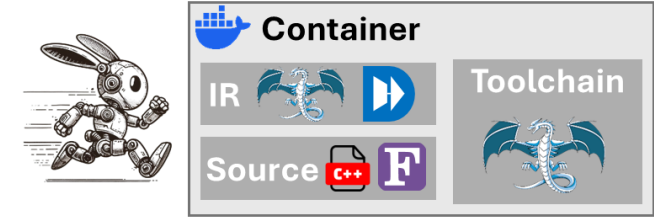
AVX-512, CUDA, MPI

Config N° 3

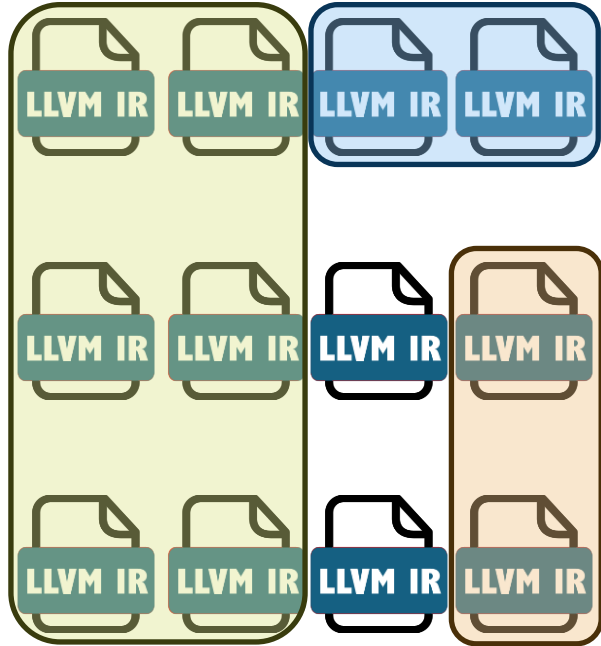
AVX-256, CUDA, MPI

- ✗ Compile-time definitions.
- ✗ Include paths in build directories.
- ✗ Vectorization and architecture flags.
- ✗ OpenMP flags.

XaaS IR Containers: Eliminating Redundancy



XaaS IR Container



Config N° 1

AVX-256, no GPU, OpenMP

Config N° 2

AVX-512, CUDA, MPI

Config N° 3

AVX-256, CUDA, MPI

- ❌ Compile-time definitions.
- ❌ Include paths in build directories.
- ❌ Vectorization and architecture flags.
- ❌ OpenMP flags.

Example 1: GROMACS, CPU Vectorization (5)

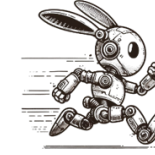
Example 2: GROMACS, CUDA + CPU Vectorization (2)








5 Build Configurations: 8710 compiled files
IR Container: 2695 IRs -> **69% reduction**

4 Build Configurations: 7052 compiled files
IR Container: 2694 IRs -> **62% reduction**

XaaS IR Containers: Build & Deploy

Container Build

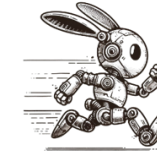
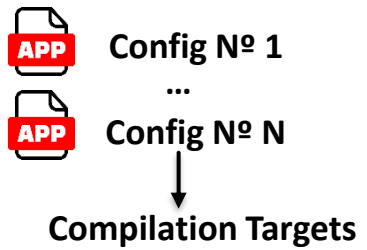









 Container	 Toolchain
IR  	
Source  	

XaaS IR Container

XaaS IR Containers: Build & Deploy

Container Build

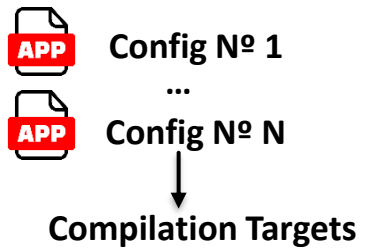


 Container	 Toolchain
IR  	
Source  	

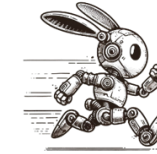
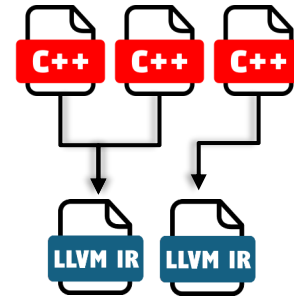
XaaS IR Container







XaaS IR Containers: Build & Deploy

Container Build



- Preprocessing
- OpenMP Detection
- Vectorization
- Building IRs

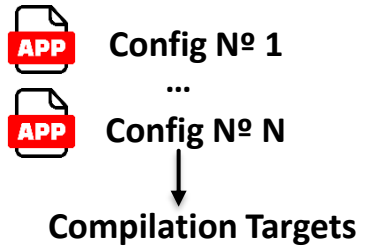


Container		Toolchain	
IR			
Source			

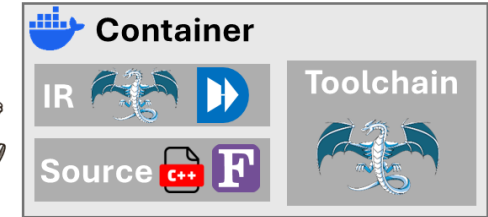
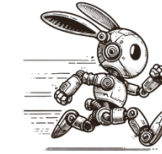
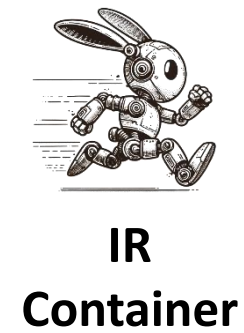
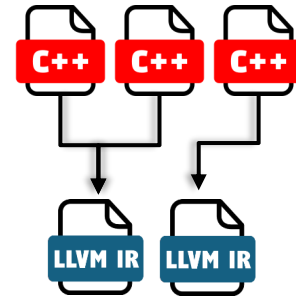
XaaS IR Container

XaaS IR Containers: Build & Deploy

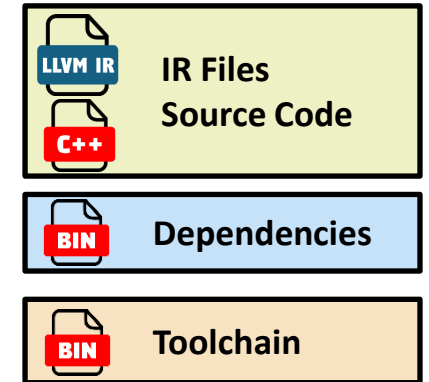
Container Build



- Preprocessing
- OpenMP Detection
- Vectorization
- Building IRs

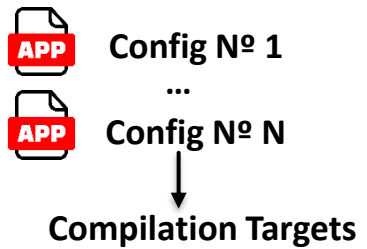


XaaS IR Container

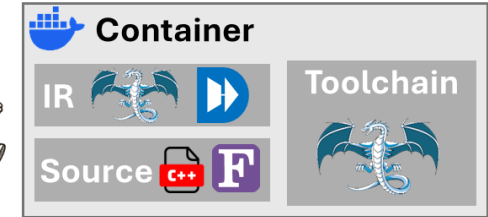
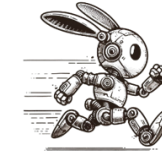
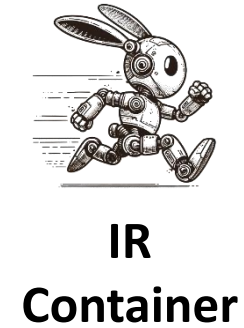
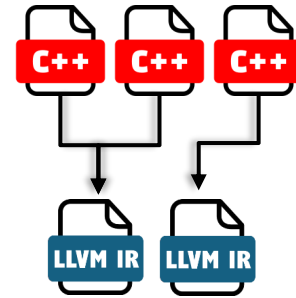


XaaS IR Containers: Build & Deploy

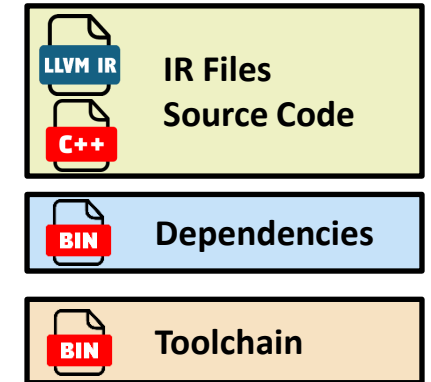
Container Build



- Preprocessing
- OpenMP Detection
- Vectorization
- Building IRs



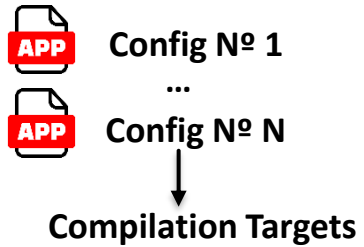
XaaS IR Container



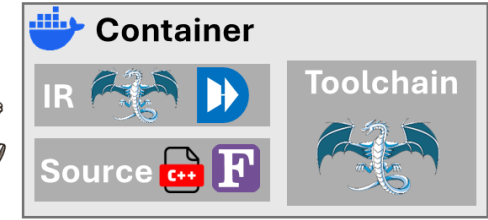
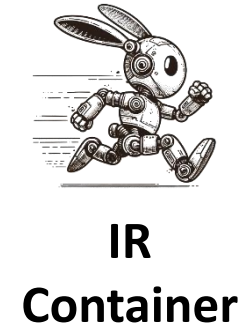
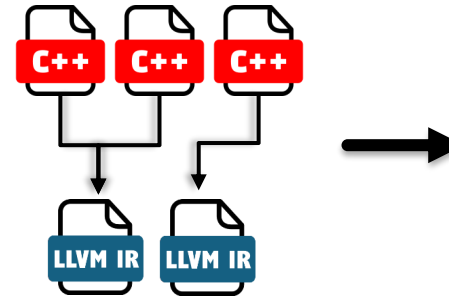
Container Deployment

XaaS IR Containers: Build & Deploy

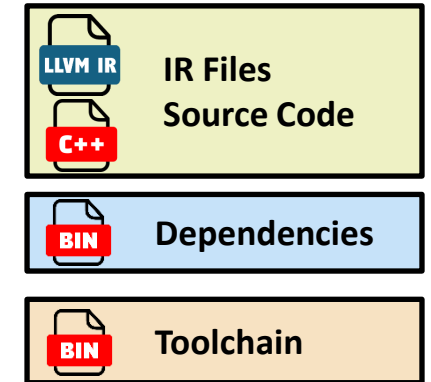
Container Build



- Preprocessing
- OpenMP Detection
- Vectorization
- Building IRs



XaaS IR Container

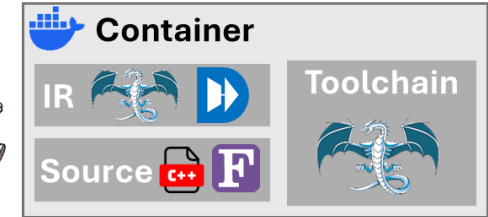
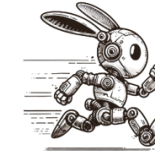


Container Deployment

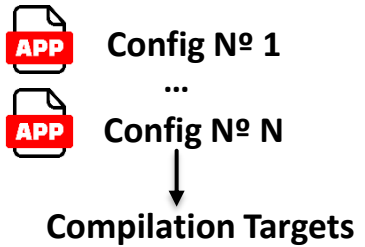


Specialization
Selection

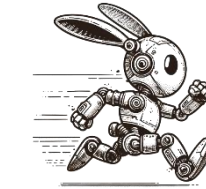
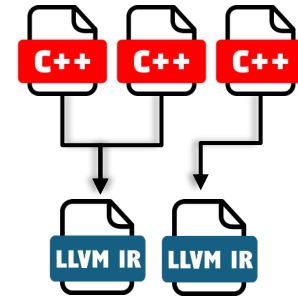
XaaS IR Containers: Build & Deploy



Container Build

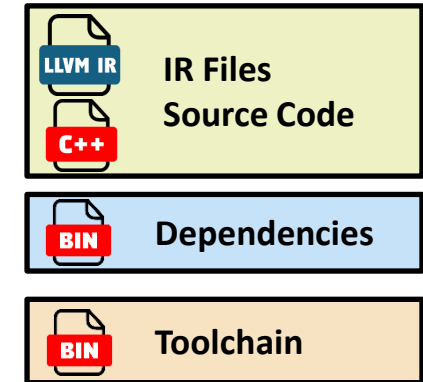


- Preprocessing
- OpenMP Detection
- Vectorization
- Building IRs



IR
Container

XaaS IR Container



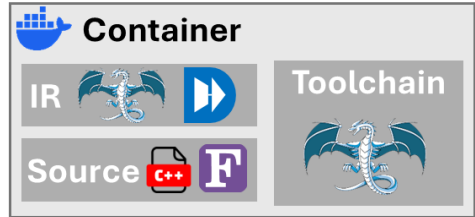
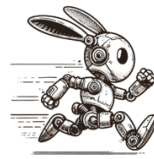
Container Deployment



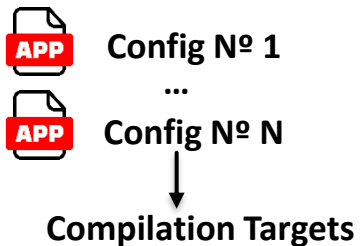
LLVM Vectorization,
Lowering

Specialization
Selection

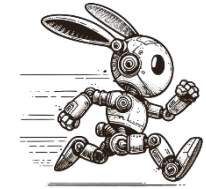
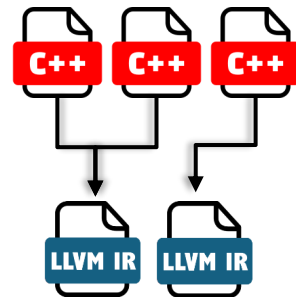
XaaS IR Containers: Build & Deploy



Container Build

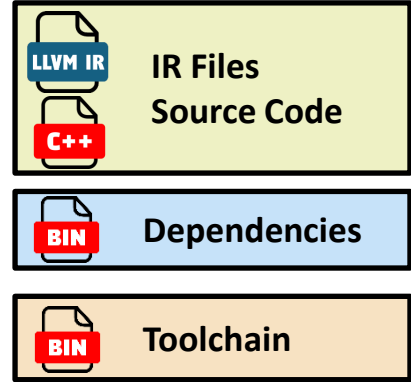


- Preprocessing
- OpenMP Detection
- Vectorization
- Building IRs



IR
Container

XaaS IR Container



Container Deployment



Specialization
Selection



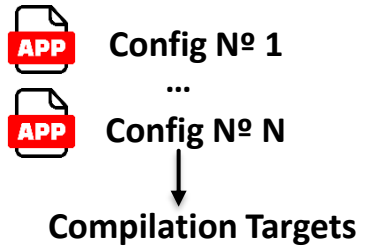
LLVM Vectorization,
Lowering



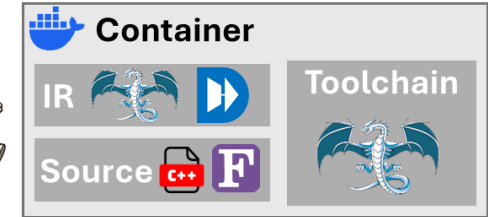
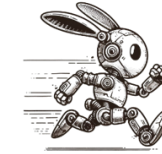
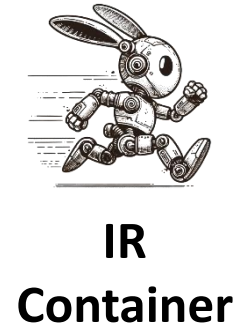
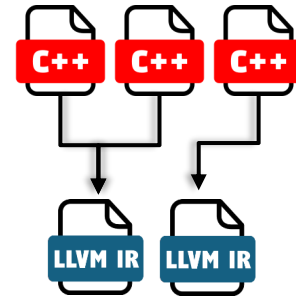
Linking,
Installation

XaaS IR Containers: Build & Deploy

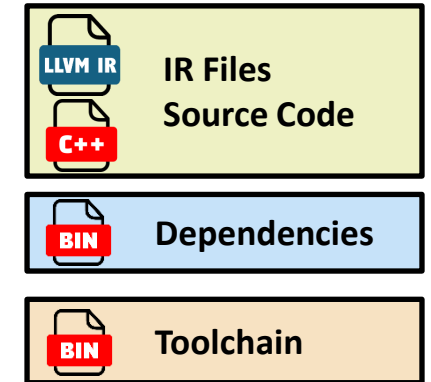
Container Build



- Preprocessing
- OpenMP Detection
- Vectorization
- Building IRs



XaaS IR Container



Container Deployment



Specialization Selection



LLVM Vectorization, Lowering



Linking, Installation



Deployed IR Container

CSCS Ault



**Intel/AMD CPU,
NVIDIA GPU**

CSCS Alps



ARM CPU, NVIDIA GPU

ALCF Aurora



Intel CPU, Intel GPU

Can XaaS Source and IR Containers provide performance portability?

Evaluation – GROMACS in XaaS Source Containers

Alps.Clariden (GH200)

Ault23 (Intel CPU, V100)

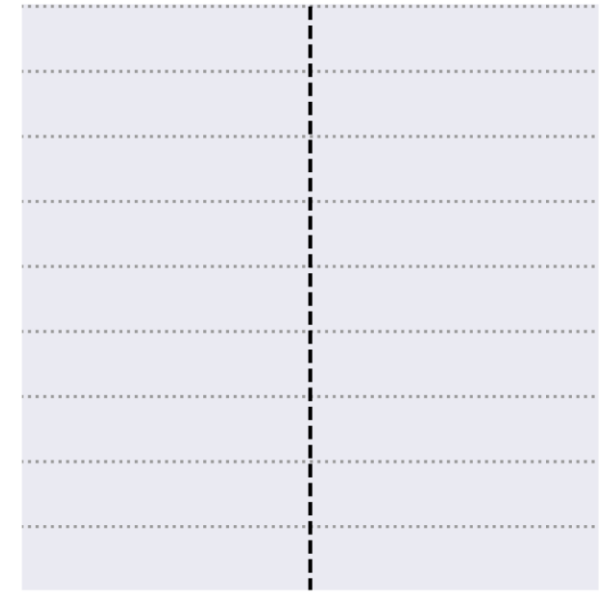
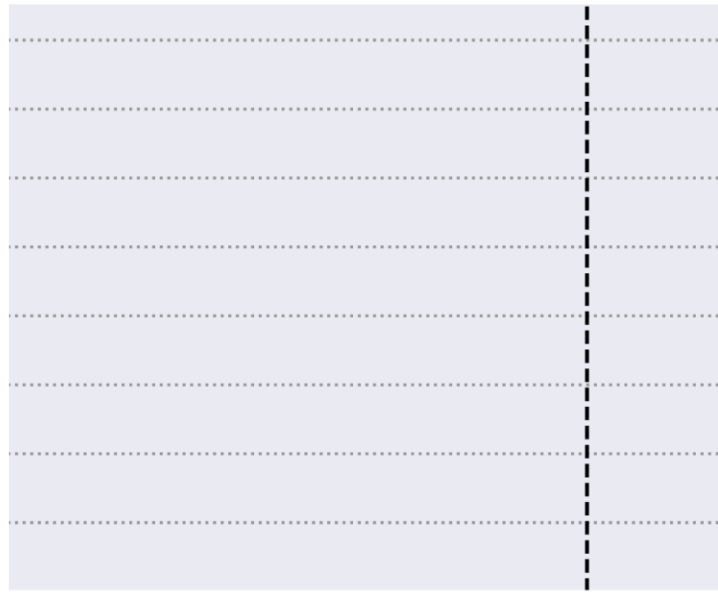
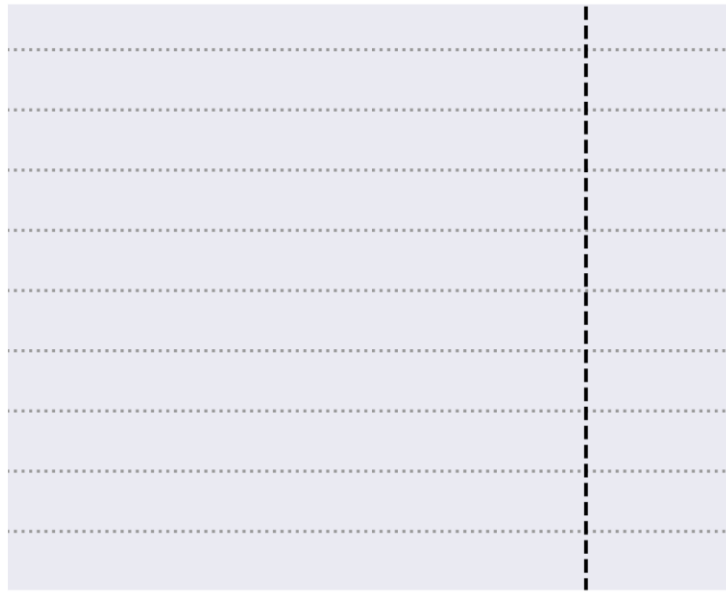
Aurora (Intel CPU + GPU)

Execution Time (s)

180
160
140
120
100
80
60
40
20

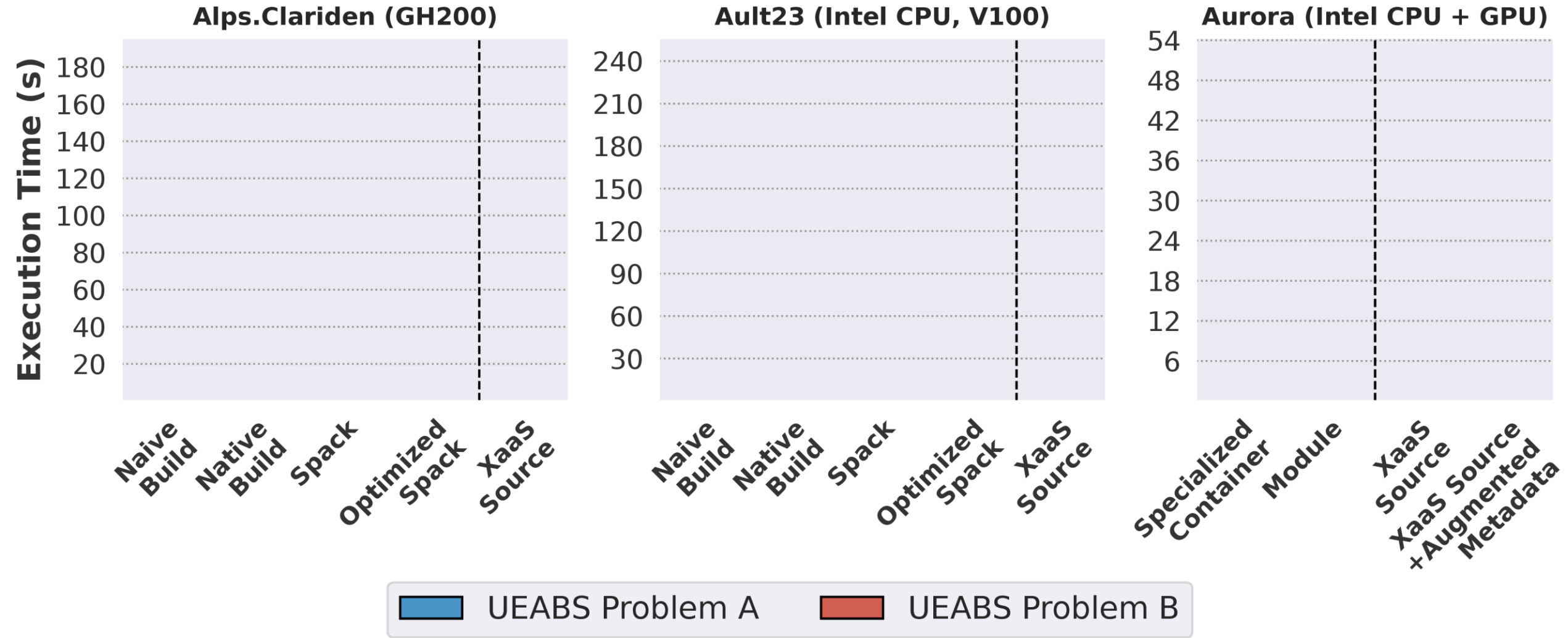
240
210
180
150
120
90
60
30

54
48
42
36
30
24
18
12
6



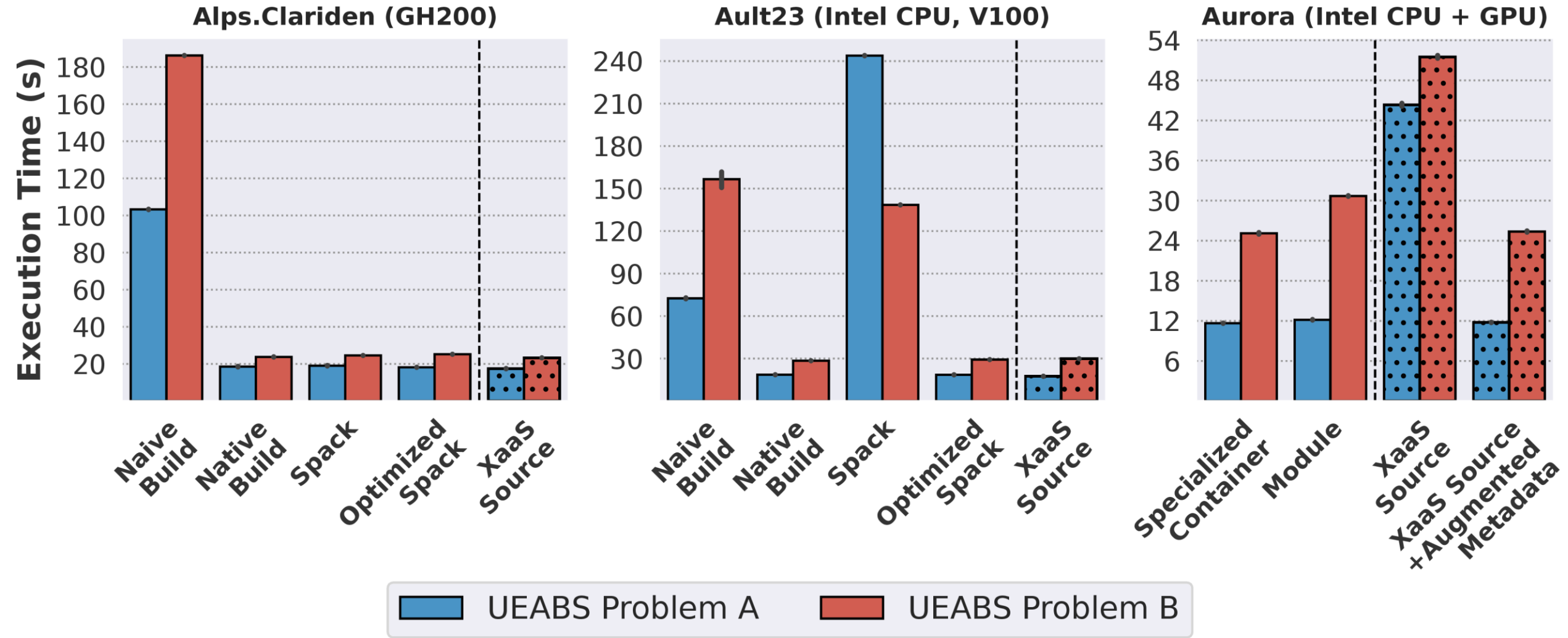
UEABS Problem A
 UEABS Problem B

Evaluation – GROMACS in XaaS Source Containers



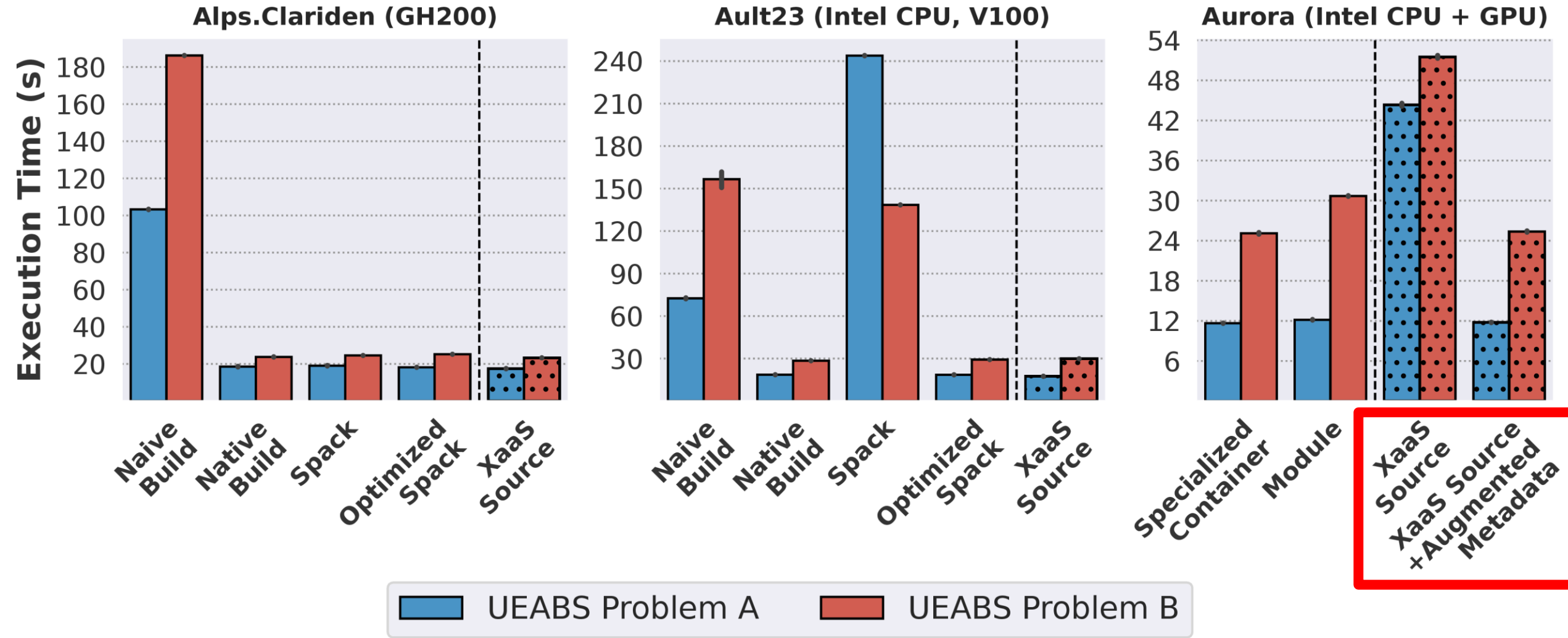
Baselines (depending on availability): “naïve” build, specialized native builds, specialized containers, system modules, Spack.

Evaluation – GROMACS in XaaS Source Containers



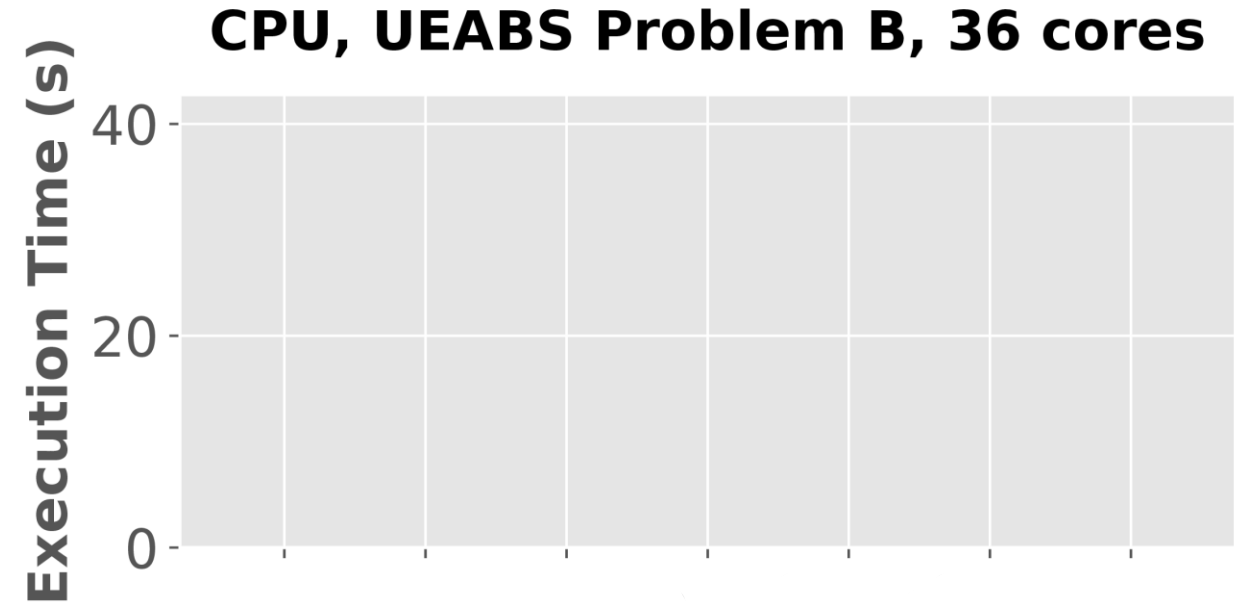
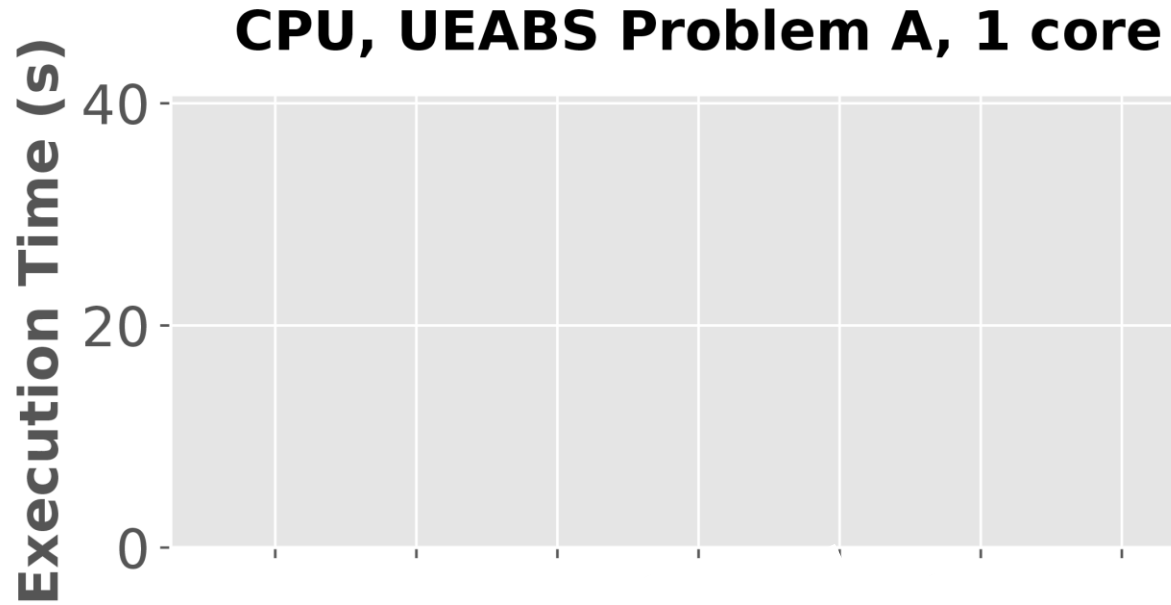
Baselines (depending on availability): “naïve” build, specialized native builds, specialized containers, system modules, Spack.

Evaluation – GROMACS in XaaS Source Containers



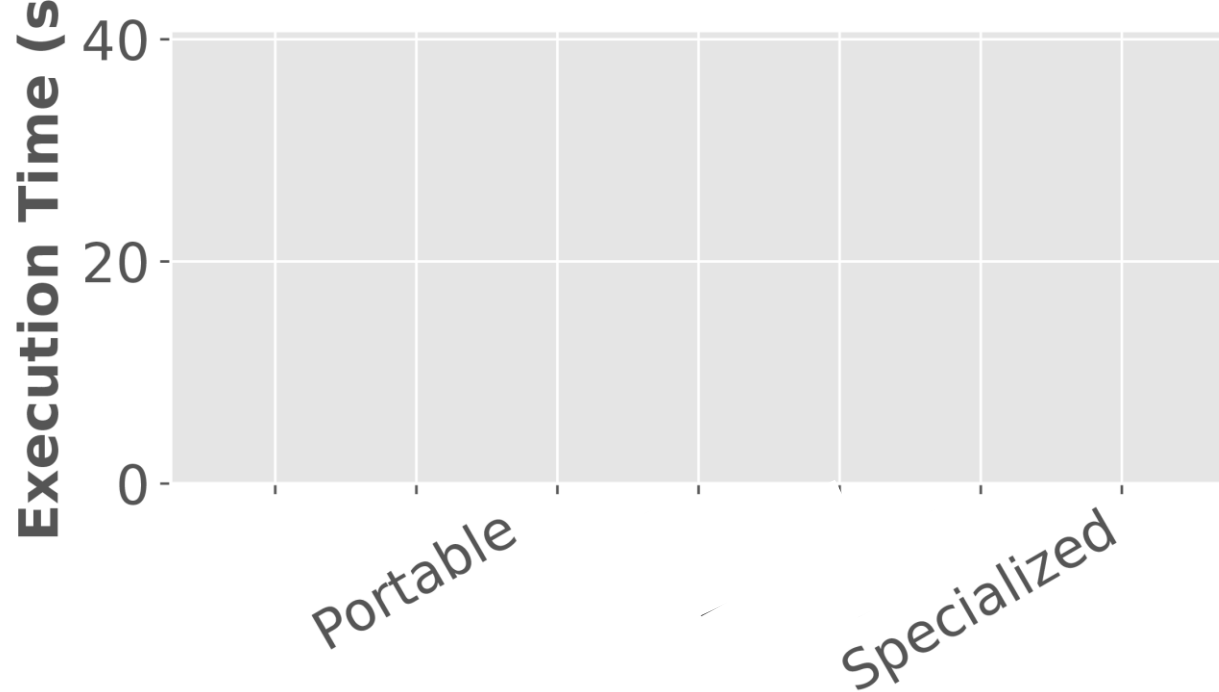
Baselines (depending on availability): “naïve” build, specialized native builds, specialized containers, system modules, Spack.

Evaluation – XaaS IR Containers with CPU Vectorization

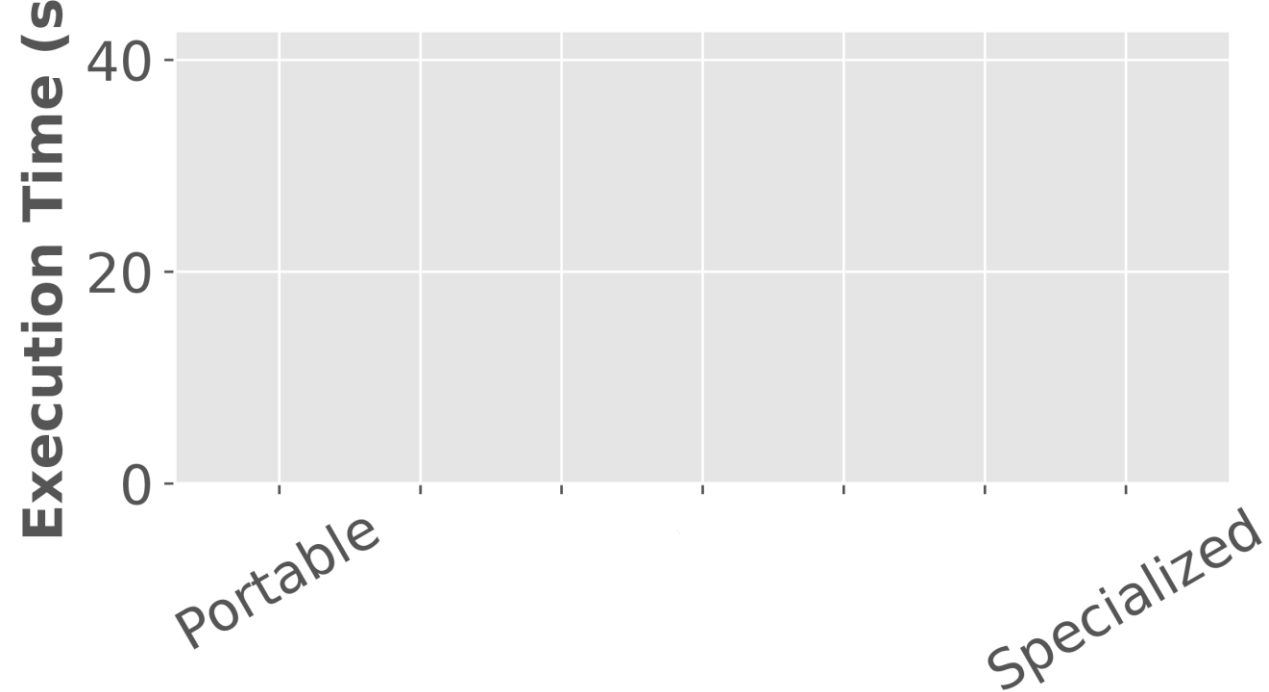


Evaluation – XaaS IR Containers with CPU Vectorization

CPU, UEABS Problem A, 1 core

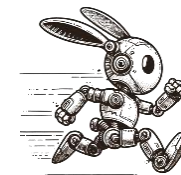
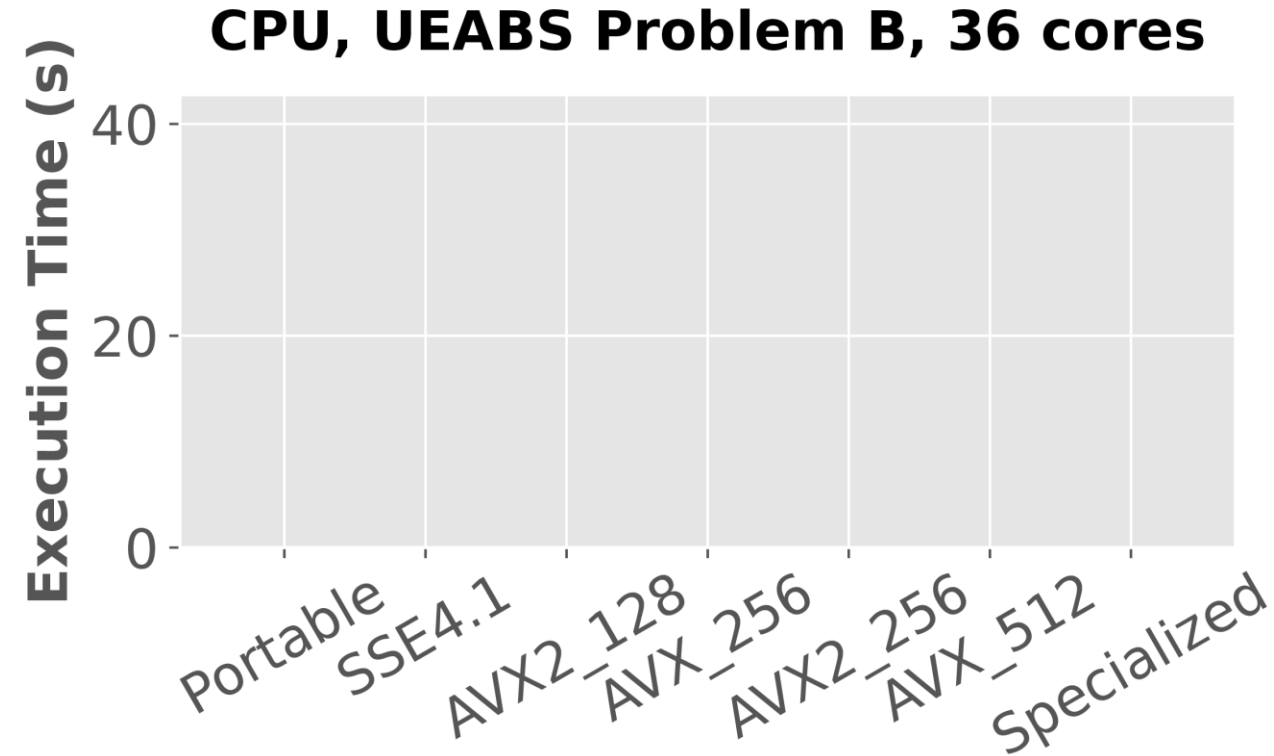
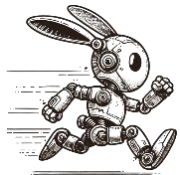
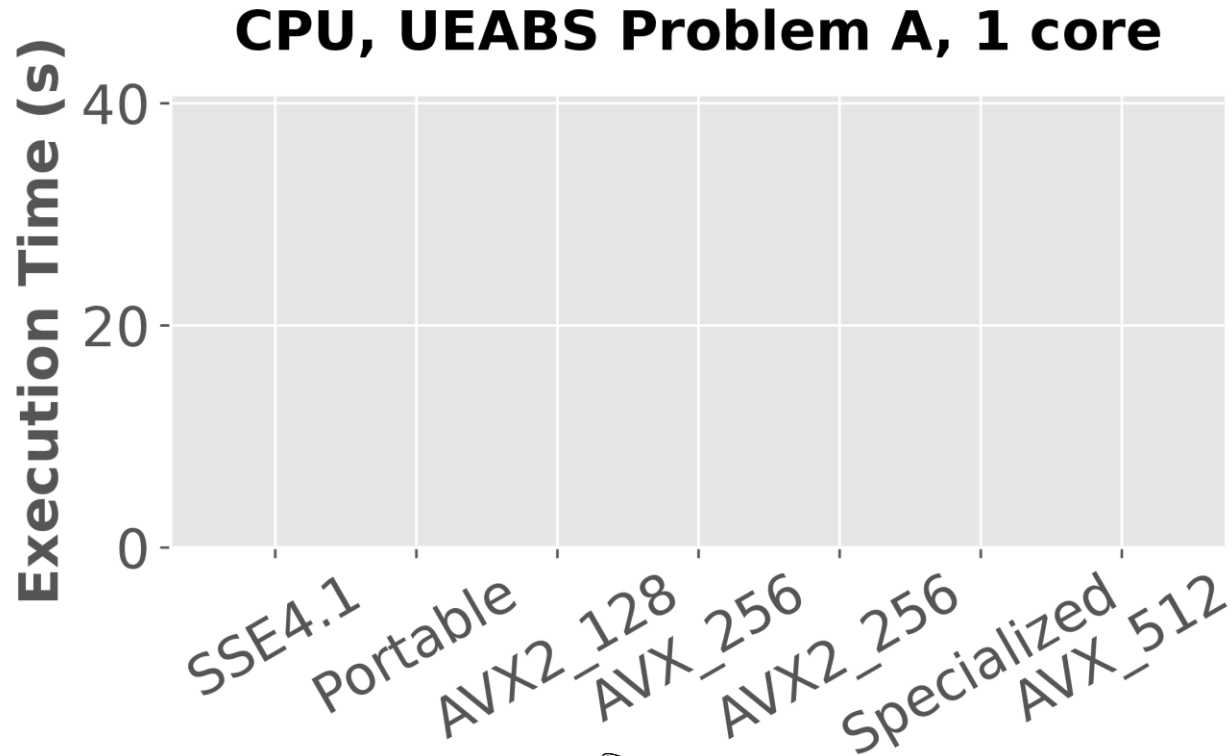


CPU, UEABS Problem B, 36 cores



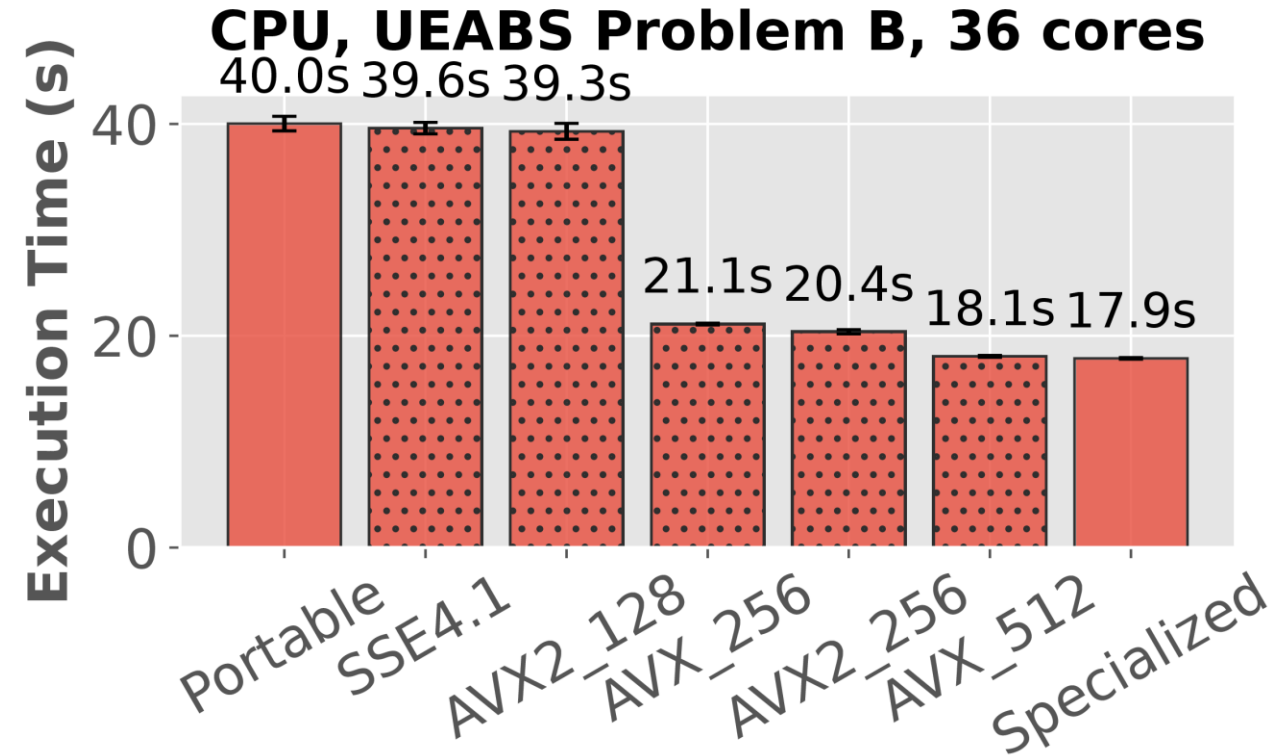
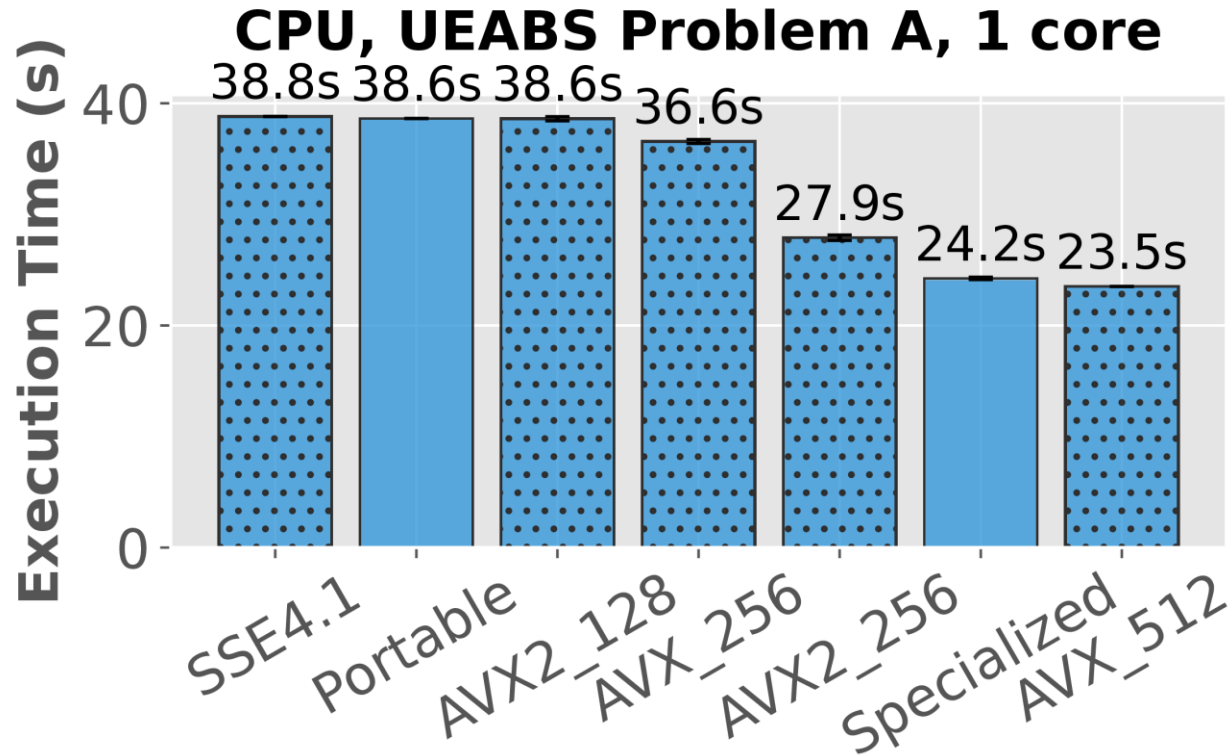
Baselines: portable (SSE4.1) and specialized (AVX-512) Docker containers.

Evaluation – XaaS IR Containers with CPU Vectorization



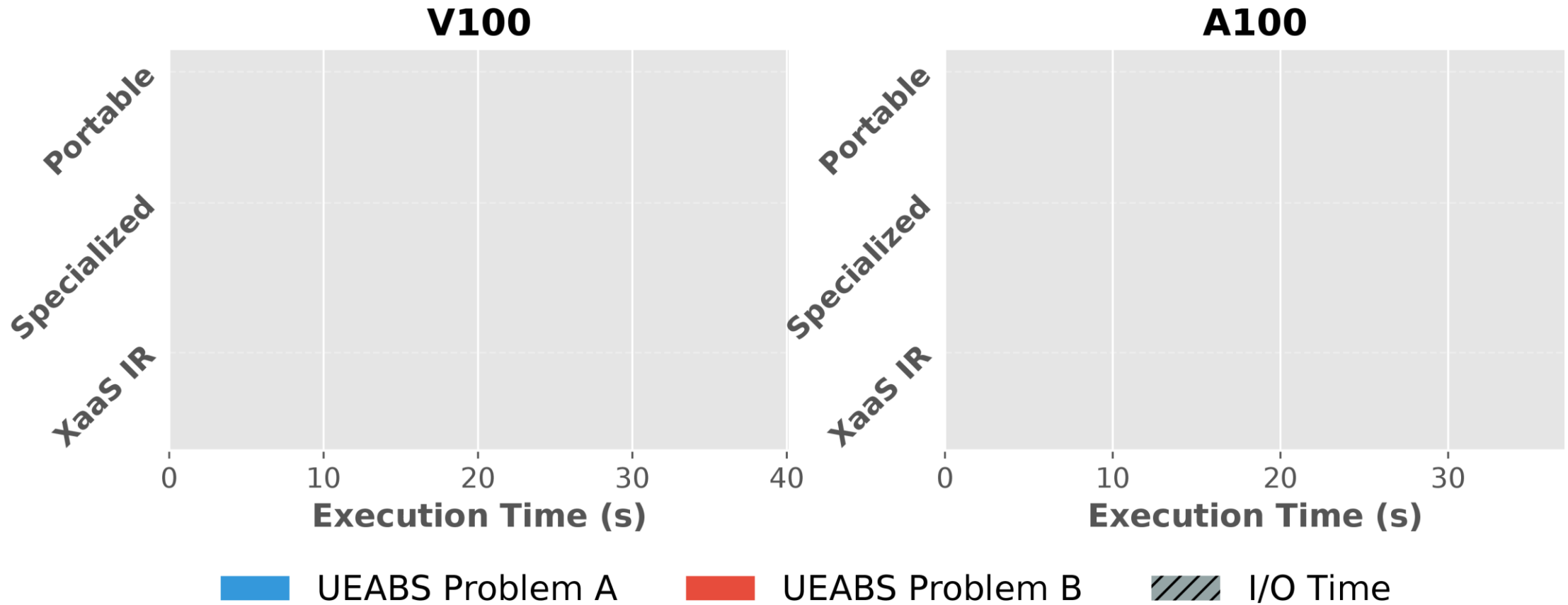
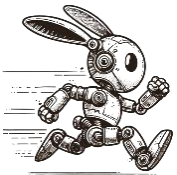
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Evaluation – XaaS IR Containers with CPU Vectorization



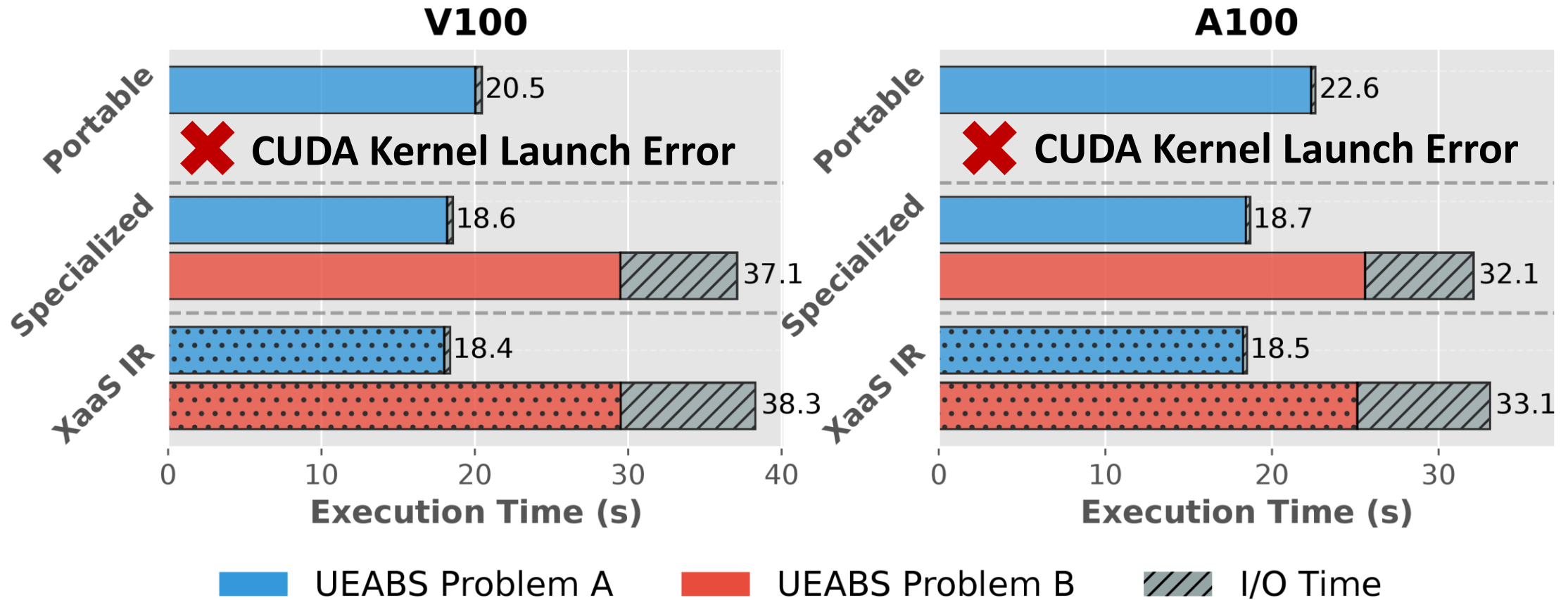
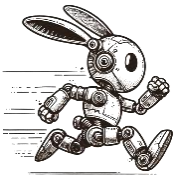
Baselines: portable (SSE4.1) and specialized (AVX-512) Docker containers.

Evaluation – XaaS IR Containers with CUDA Support



Baselines: specialized Docker containers with CUDA, AVX-512 (V100) or AVX-256 (A100).
 Portable containers with SYCL + CUDA, compiled with Intel's icpx compiler.

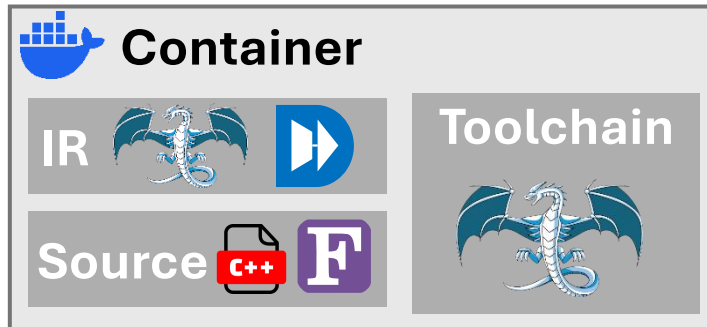
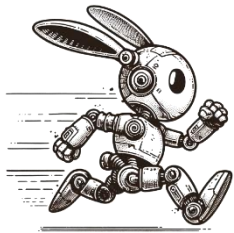
Evaluation – XaaS IR Containers with CUDA Support



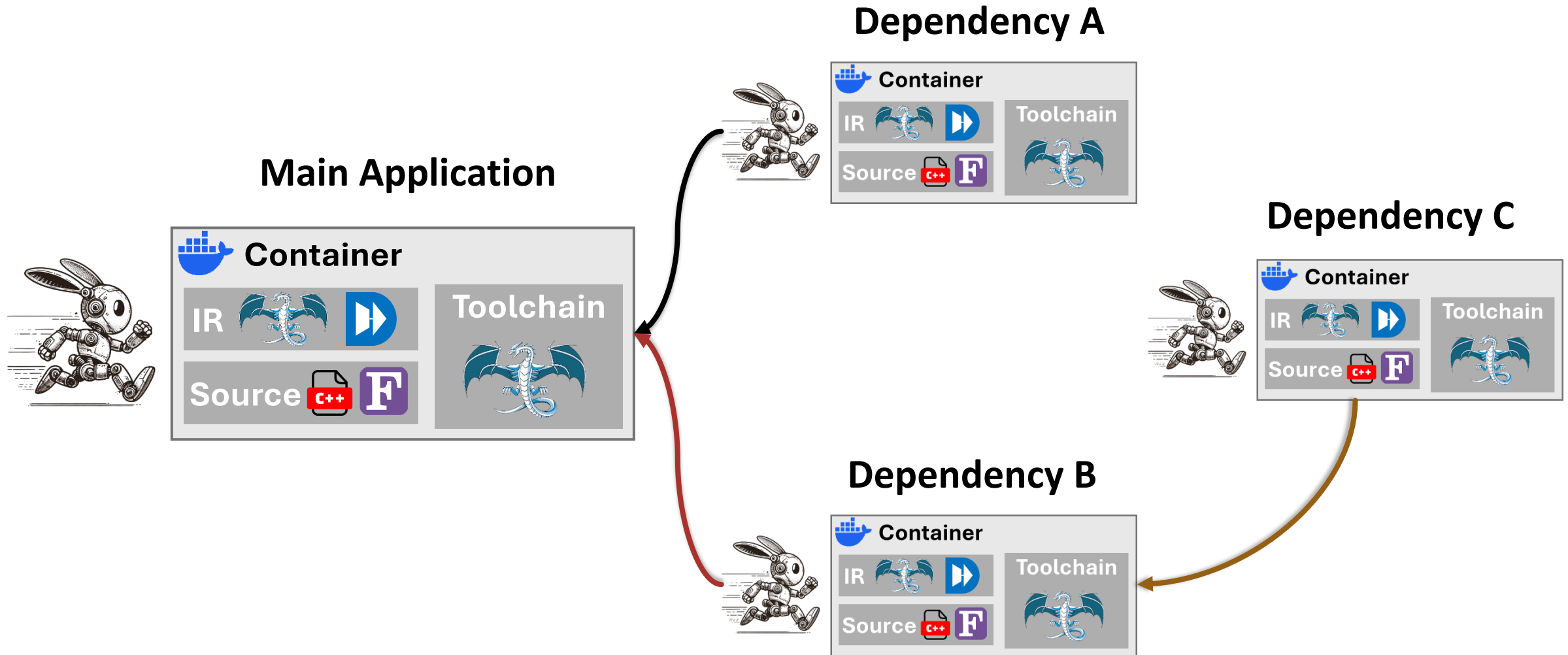
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Where Do We Go Next?

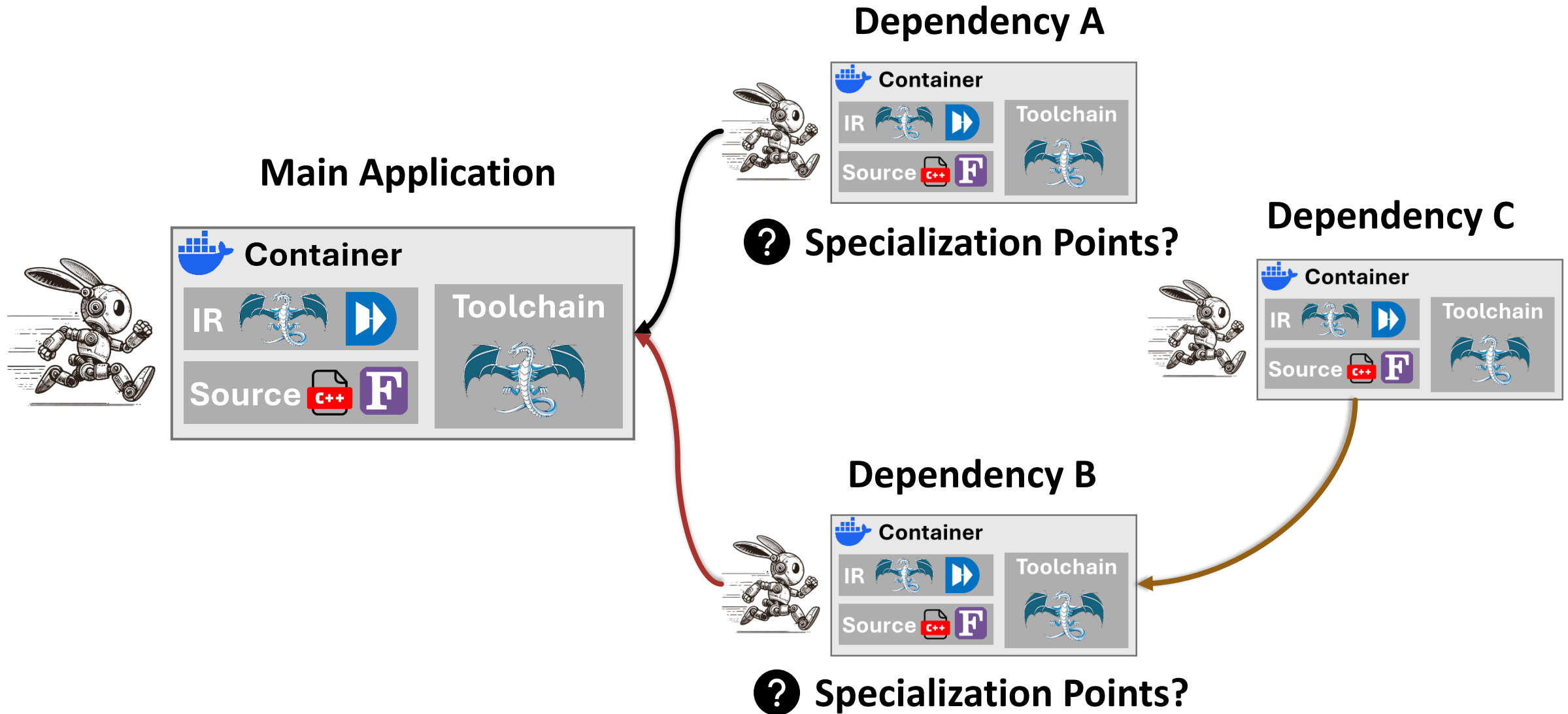
Main Application



Where Do We Go Next?



Where Do We Go Next?



Where Do We Go Next?

(1) Which build configurations matter the most?

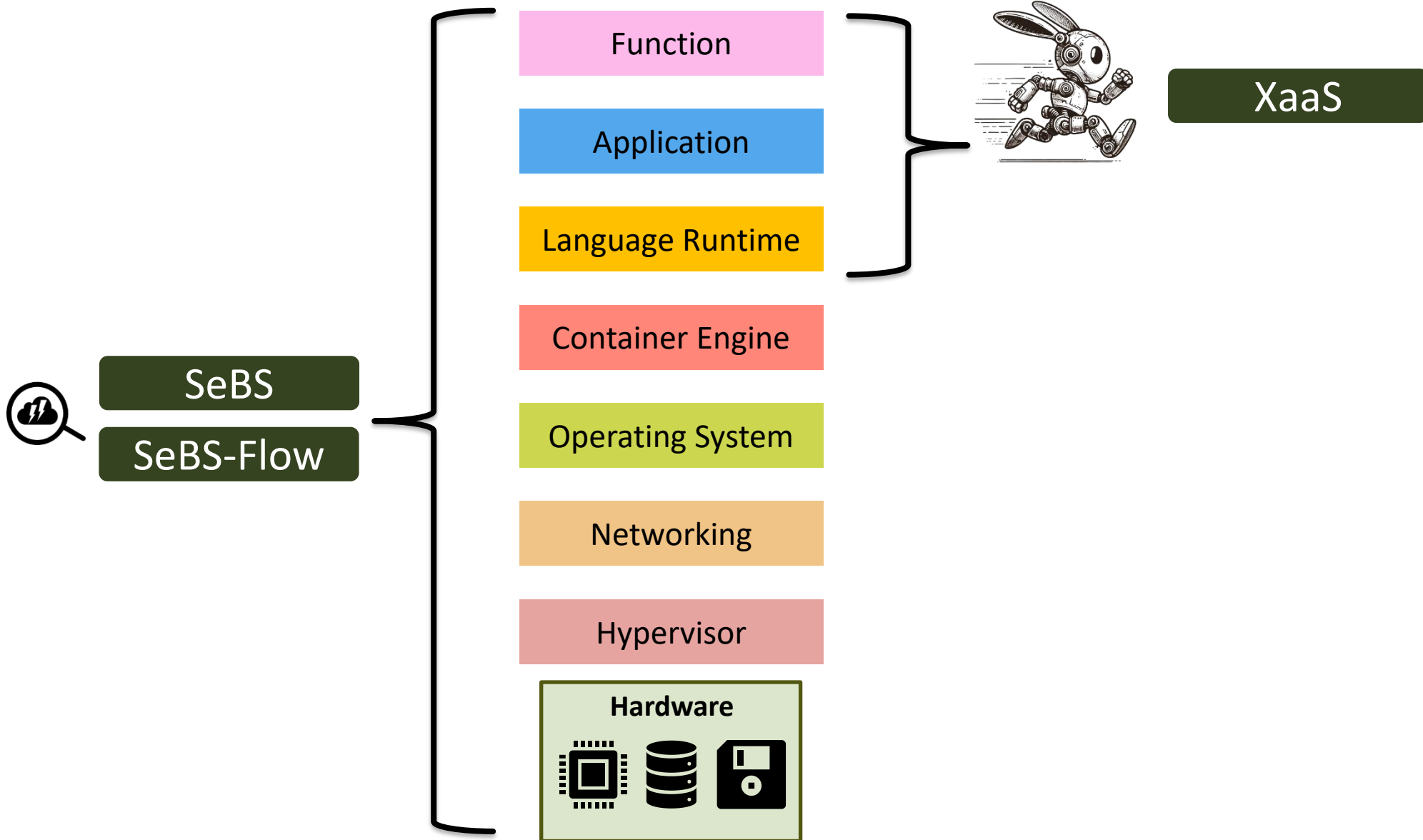
(2) Which software is not worth a rebuild?



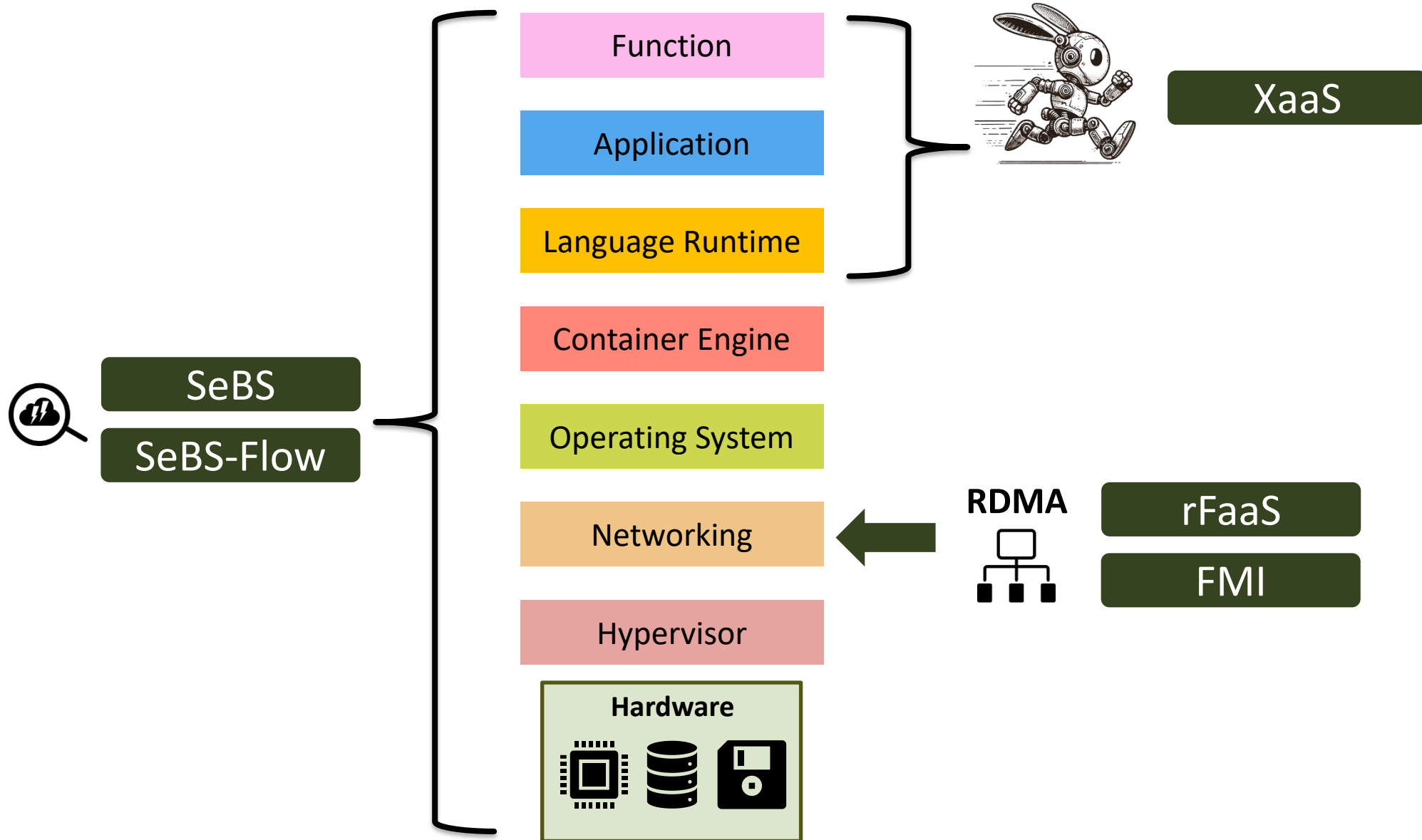
spcl/XaaS-Containers

 Specialization Points?

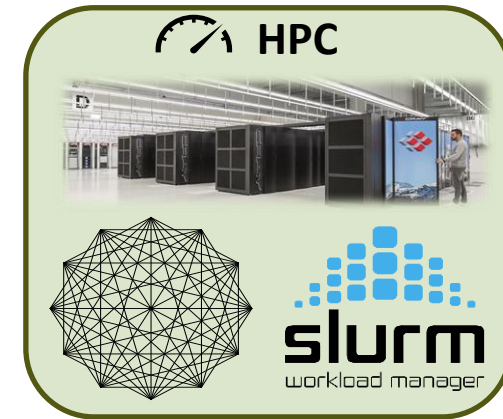
AXelerating Serverless Computing: Communicate!



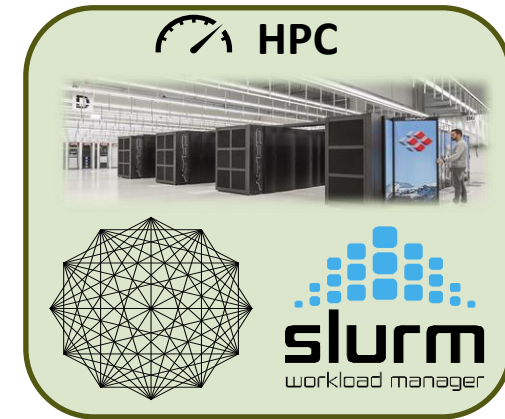
AXelerating Serverless Computing: Communicate!



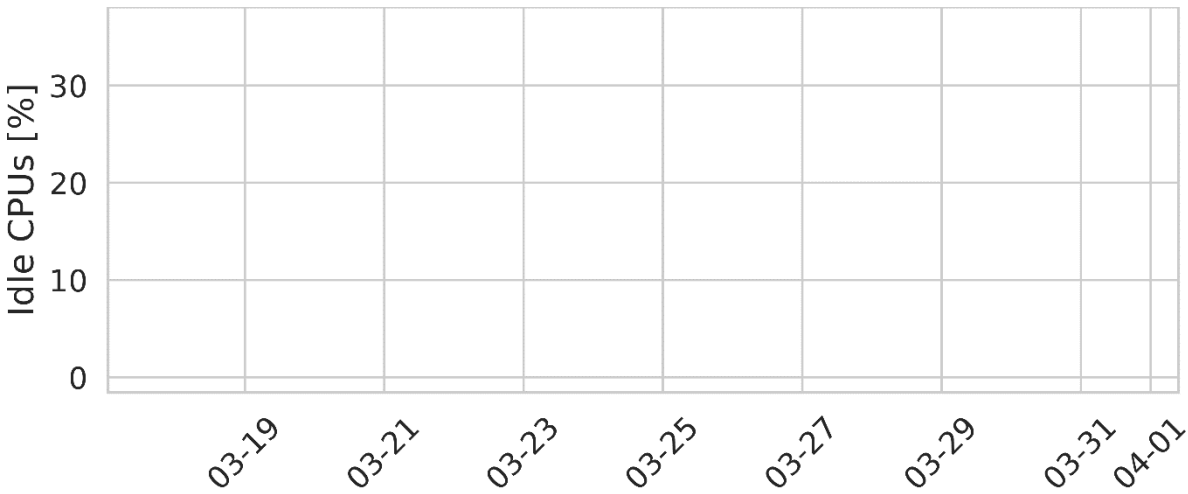
Tracking Wasted Resources in HPC



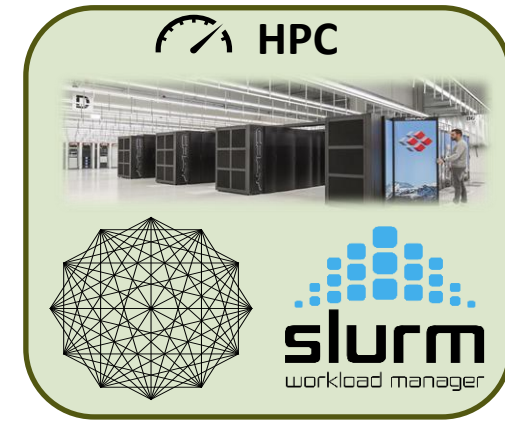
Tracking Wasted Resources in HPC



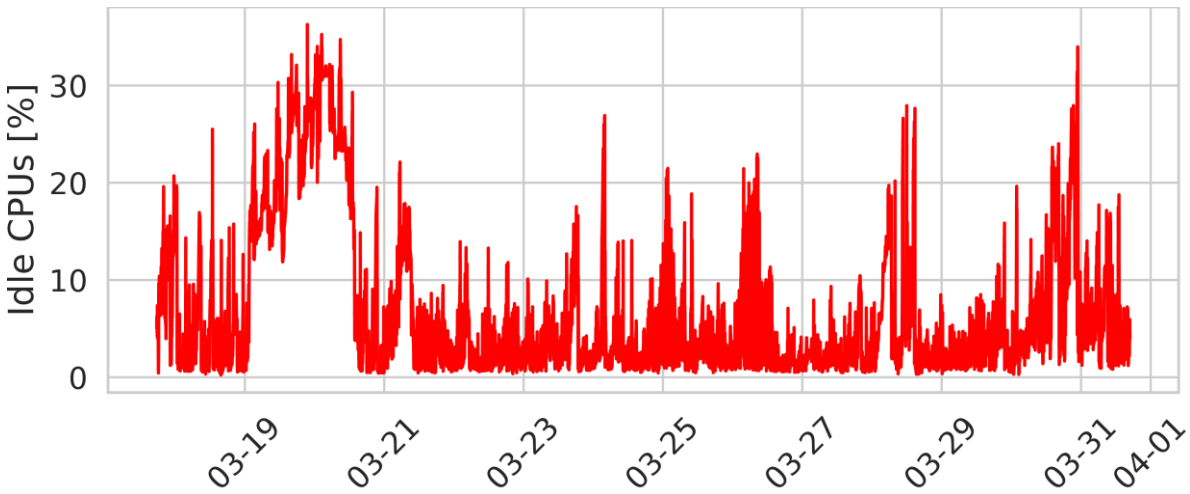
CPU



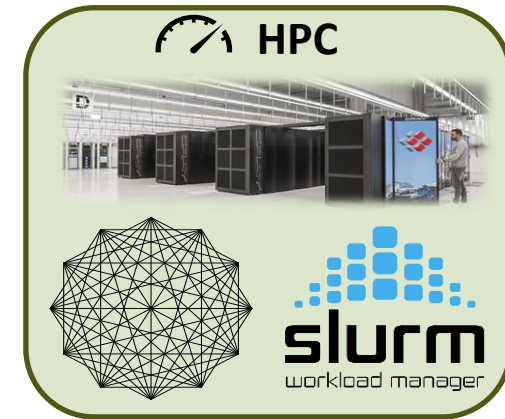
Tracking Wasted Resources in HPC



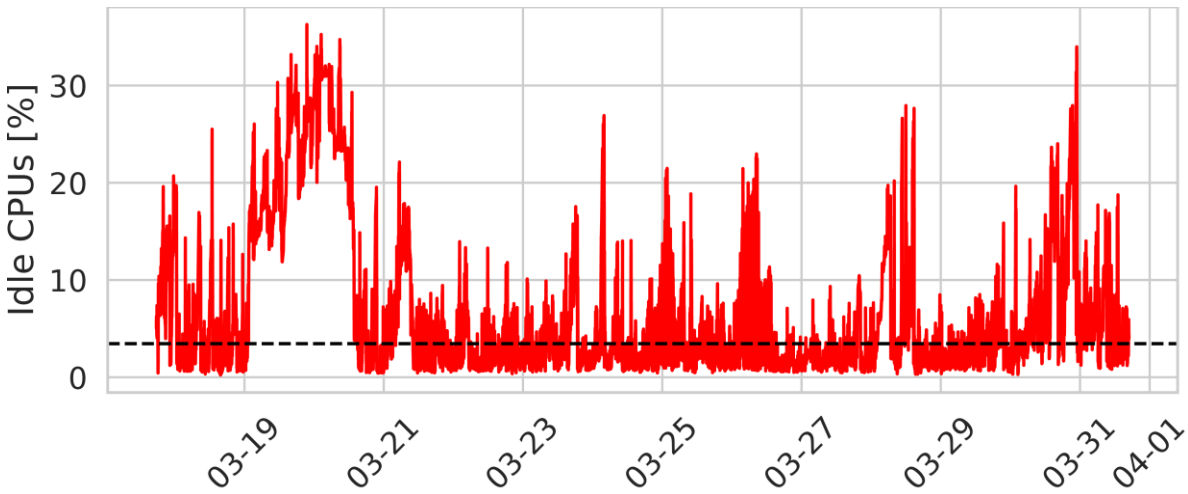
CPU



Tracking Wasted Resources in HPC

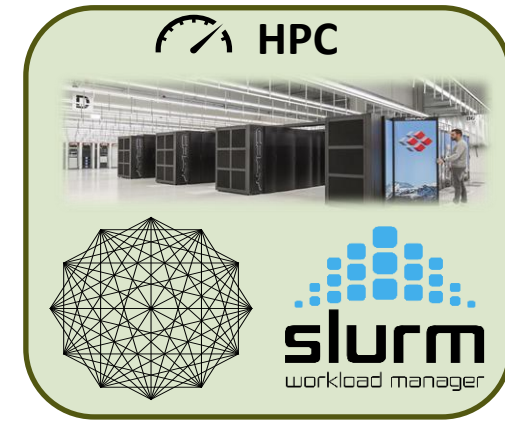


CPU

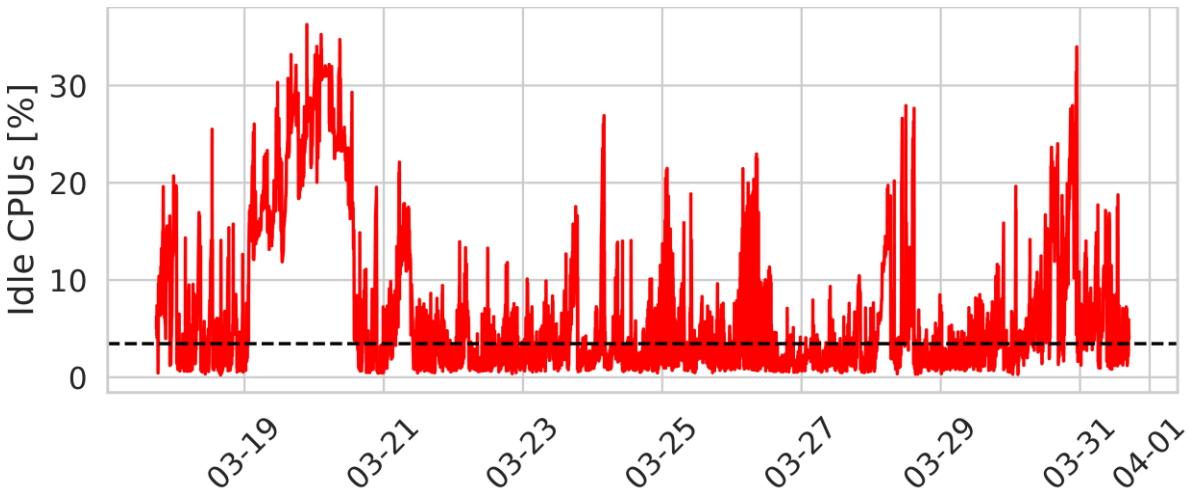


Mean idle CPUs: 6.6%

Tracking Wasted Resources in HPC

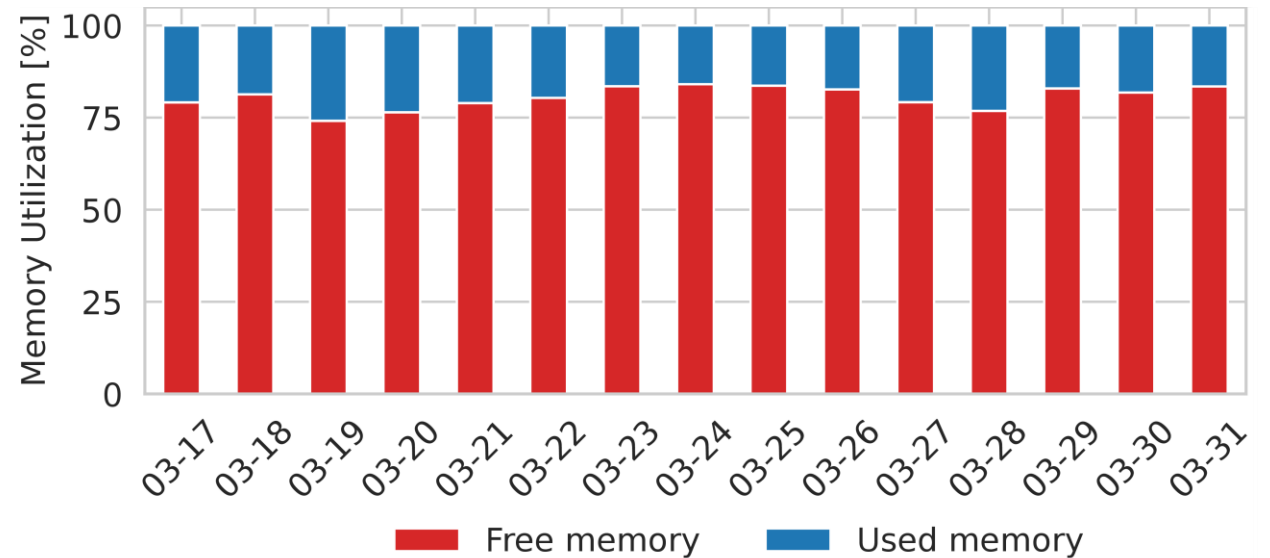


CPU



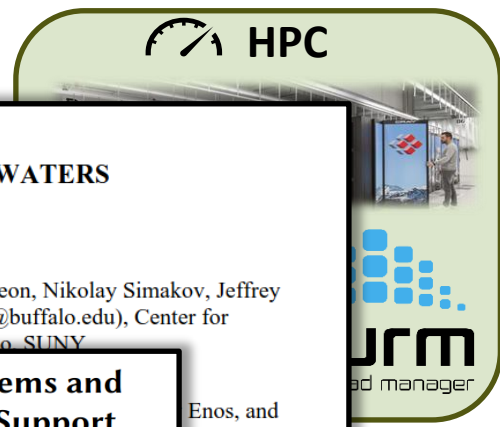
Mean idle CPUs: 6.6%

Memory



Mean free memory: 80.5%

Tracking Wasted Resources in HPC



Learning from Five-year Resource-Utilization Data of Titan System

Feiyi Wang*, Sarp Oral†, Satyabrata Sen ‡ and Neena Imam§

Oak Ridge National Laboratory

CLUSTER, 2019

FINAL REPORT
WORKLOAD ANALYSIS OF BLUE WATERS
(ACI 1650758)

Matthew D. Jones, Joseph P. White, Martins Innus, Robert L. DeLeon, Nikolay Simakov, Jeffrey T. Palmer, Steven M. Gallo, and Thomas R. Furlani (furlani@buffalo.edu), Center for Computational Research, University at Buffalo, SUNY

Quantifying Memory Underutilization in HPC Systems and Using it to Improve Performance via Architecture Support

Gagandeep Panwar* Virginia Tech Blacksburg, USA gpanwar@vt.edu	Da Zhang* Virginia Tech Blacksburg, USA daz3@vt.edu	Yihan Pang* Virginia Tech Blacksburg, USA pyihan1@vt.edu
Mai Dahshan Virginia Tech Blacksburg, USA mdahshan@vt.edu	Nathan DeBardeleben Los Alamos National Laboratory Los Alamos, USA ndebar@lanl.gov	Binoy Ravindran Virginia Tech Blacksburg, USA binoy@vt.edu
	Xun Jian Virginia Tech Blacksburg, USA xunj@vt.edu	

MICRO, 2019

A Case For Intra-rack Resource Disaggregation in HPC

GEORGE MICHELOGIANNAKIS, Lawrence Berkeley National Laboratory, USA
BENJAMIN KLENK, NVIDIA, USA
BRANDON COOK, Lawrence Berkeley National Laboratory, USA
MIN YEE
LARRY D
KEREN
JOHN S

A Holistic View of Memory Utilization on HPC Systems: Current and Future Trends

Ivy B. Peng* peng8@llnl.gov Lawrence Livermore National Laboratory USA	Ian Karlin karlin1@llnl.gov Lawrence Livermore National Laboratory USA	Maya B. Gokhale gokhale2@llnl.gov Lawrence Livermore National Laboratory USA
Kathleen Shoga Shoga1@llnl.gov Lawrence Livermore National Laboratory USA	Matthew Legendre legendre1@llnl.gov Lawrence Livermore National Laboratory USA	Todd Gamblin gamblin2@llnl.gov Lawrence Livermore National Laboratory USA

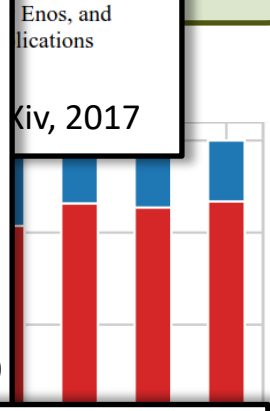
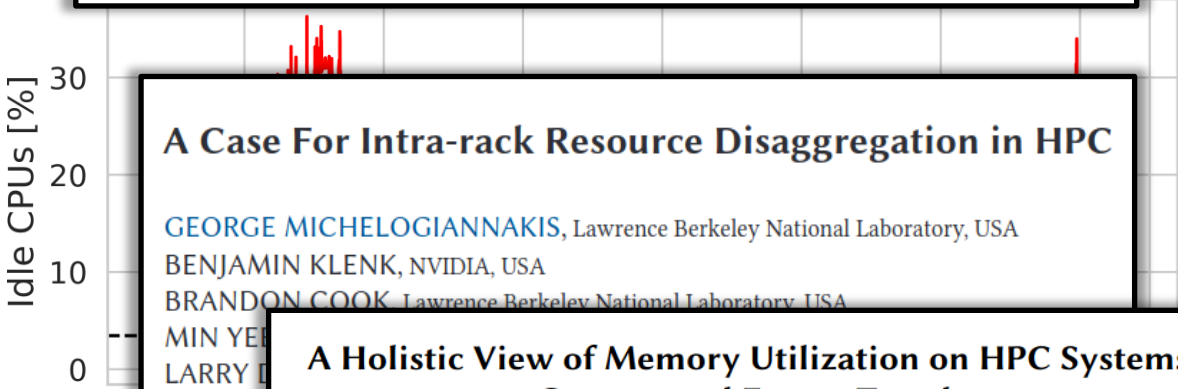
MEMSYS, 2021

Comprehensive Workload Analysis and Modeling of a Petascale Supercomputer

Haihang You¹ and Hao Zhang²

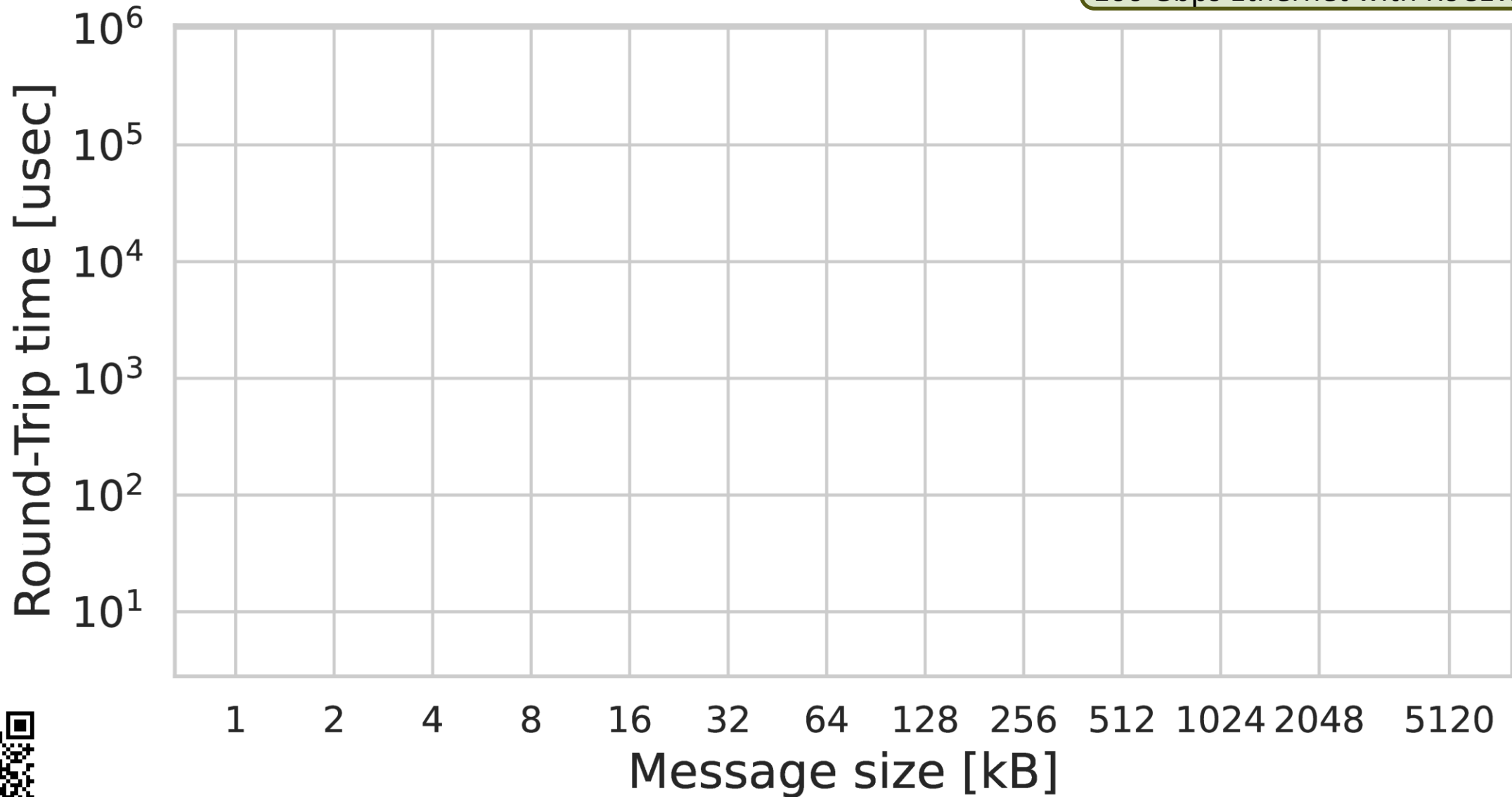
¹ National Institute for Computational Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA
² Department of Electrical Engineering and Computer Science, University of Tennessee, Knoxville, TN 37996, USA
{hyou, haozhang}@utk.edu

JSSPP, 2012



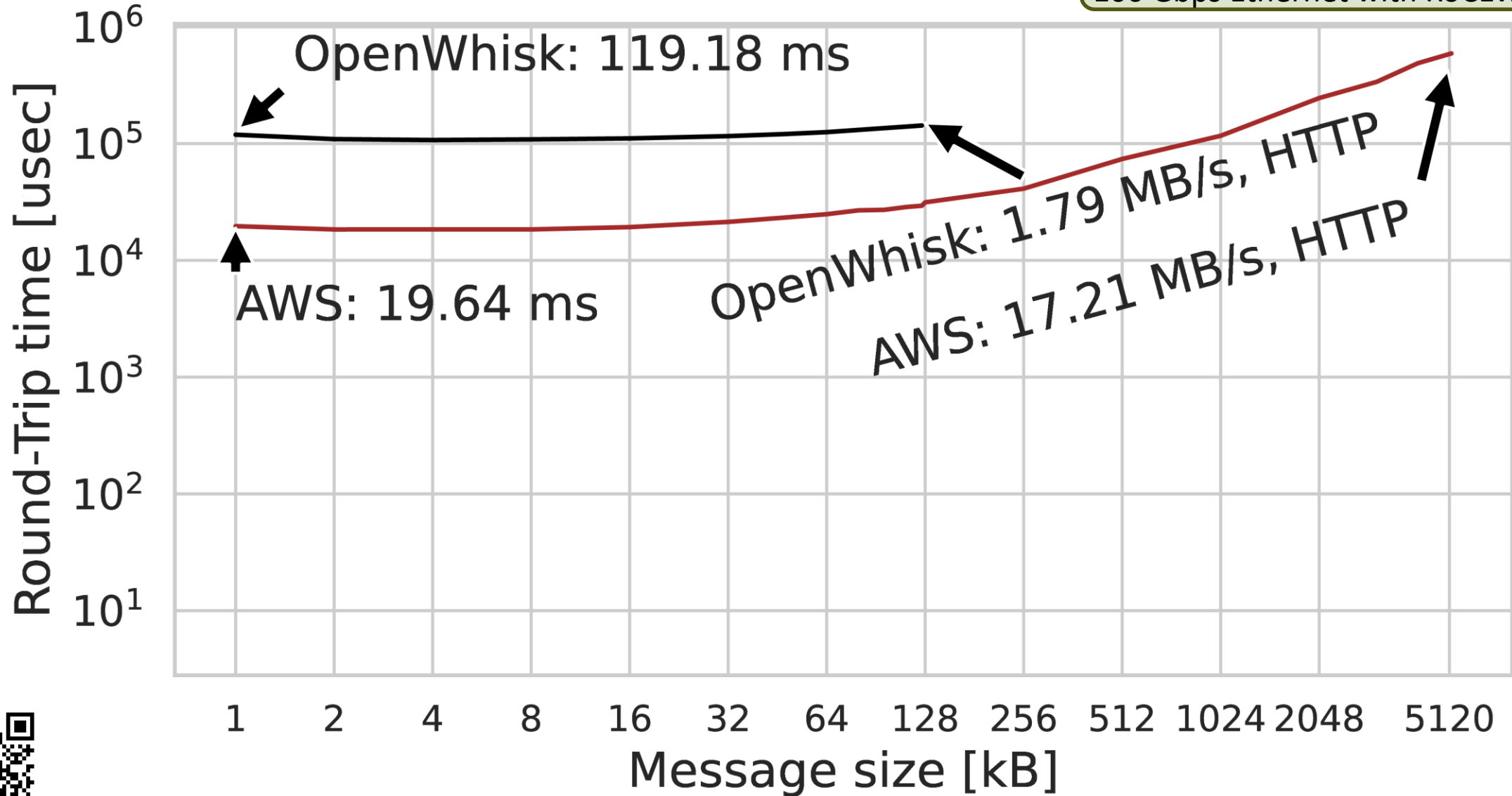
rFaaS: How Fast are Invocations in FaaS?

36 CPU cores, 377 GB memory.
100 Gbps Ethernet with RoCEv2 support.



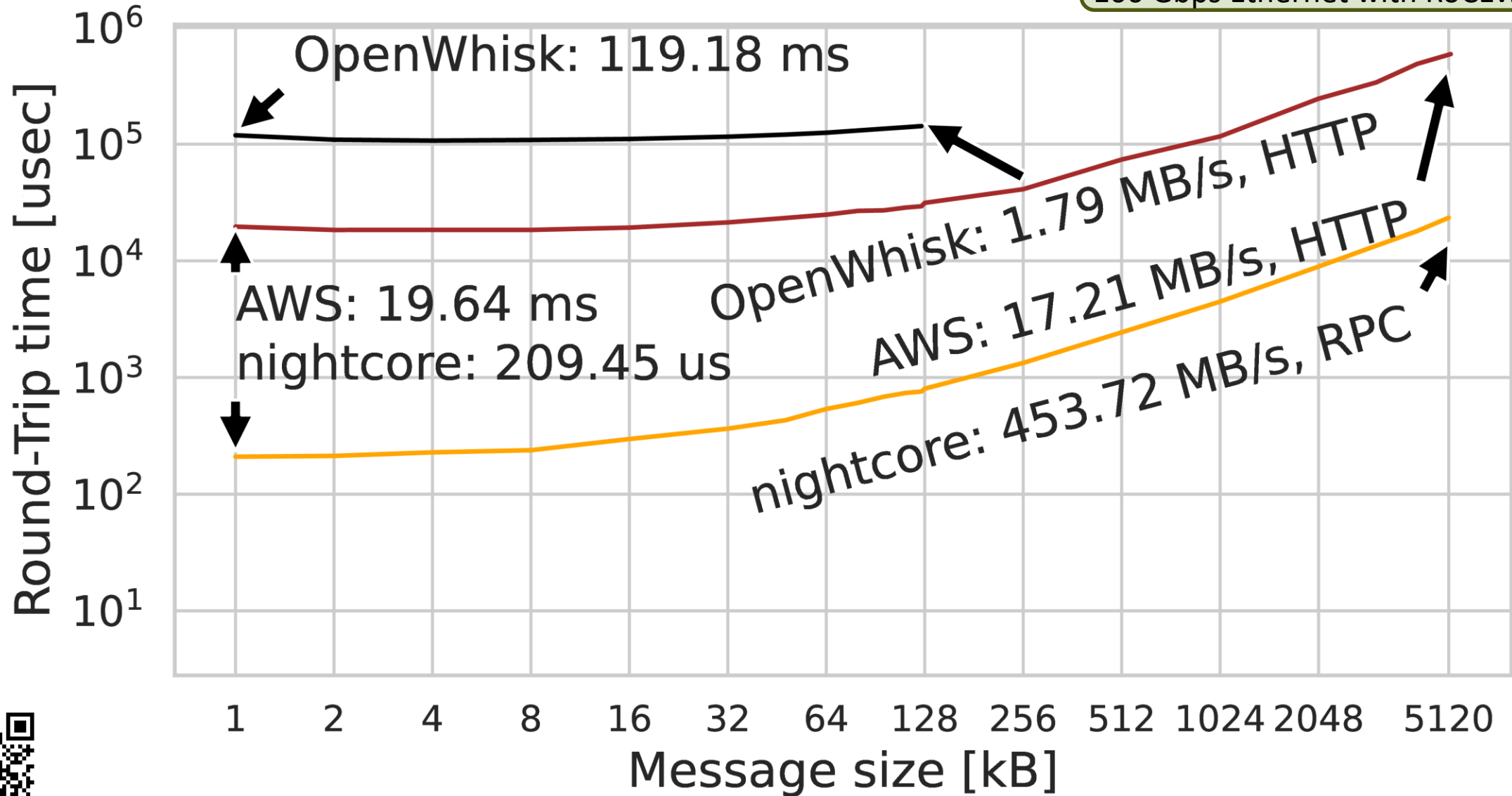
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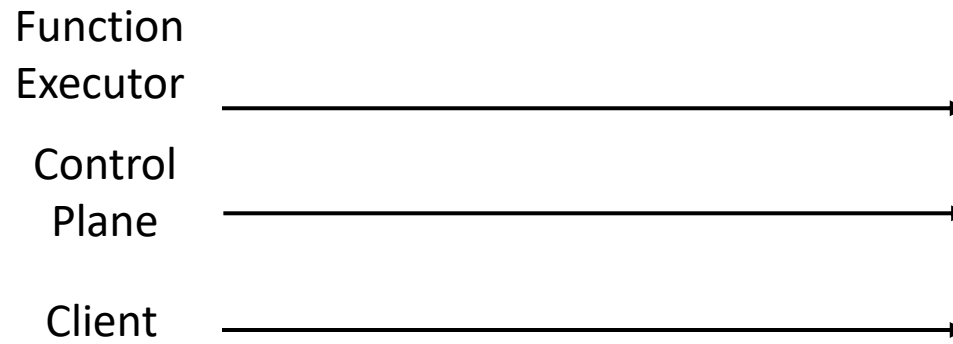


rFaaS: How Fast are Invocations in FaaS?

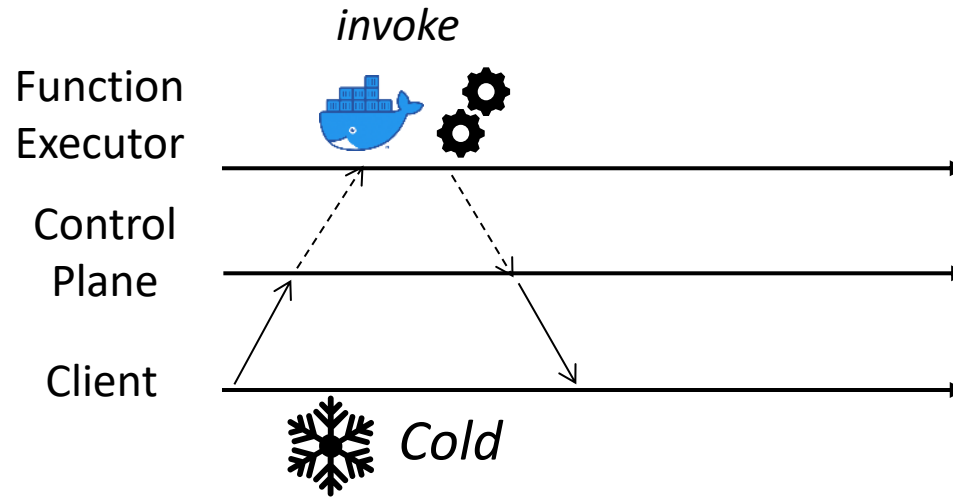
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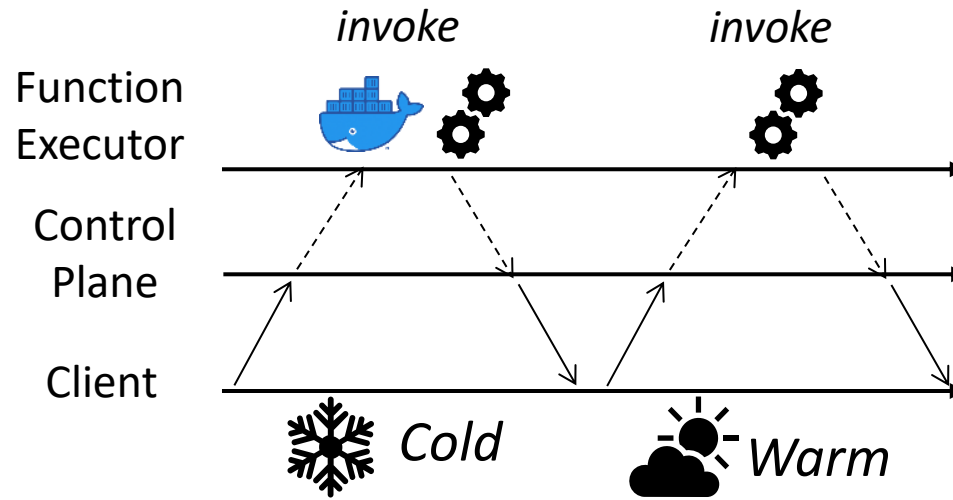
rFaaS: Invocations with Leases



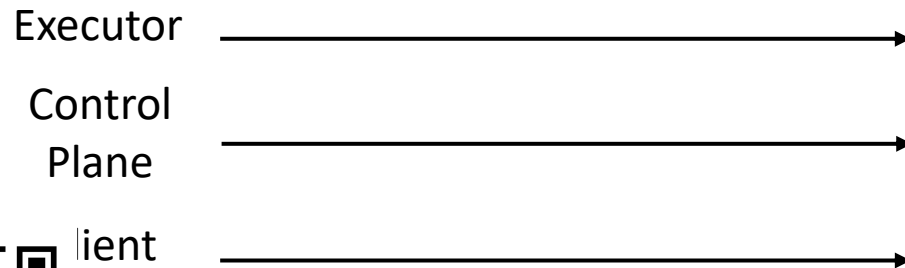
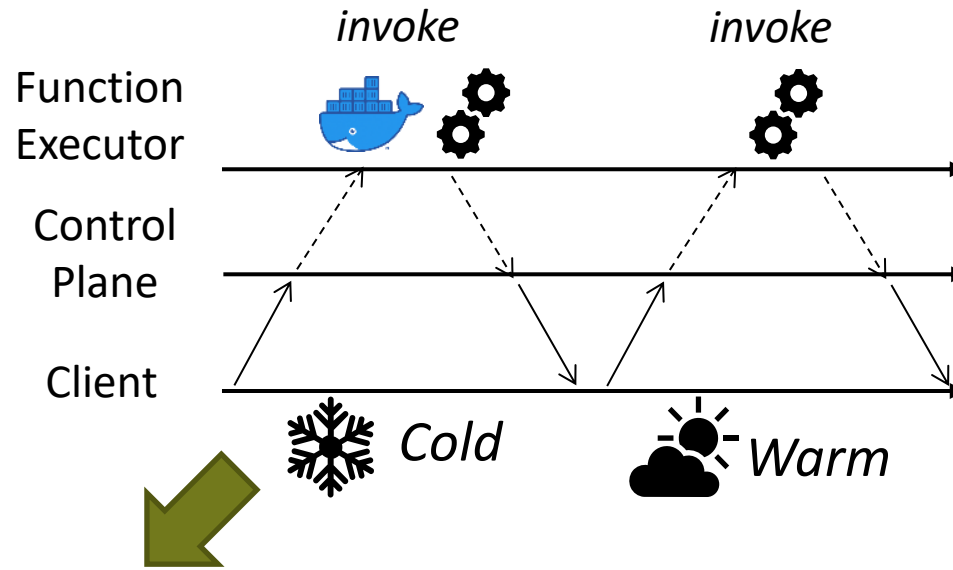
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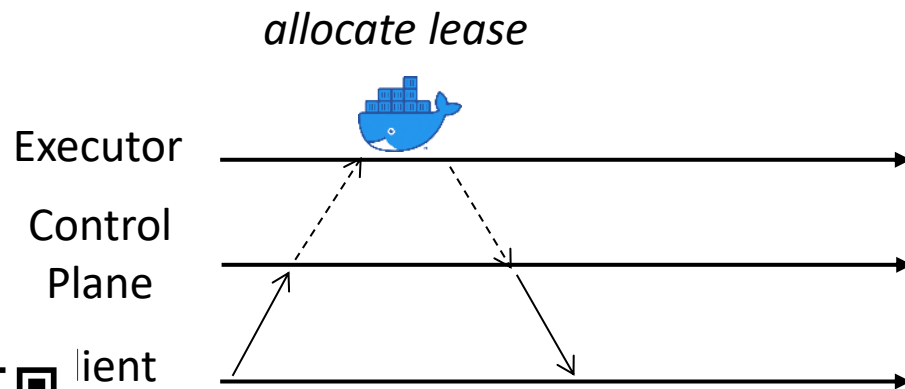
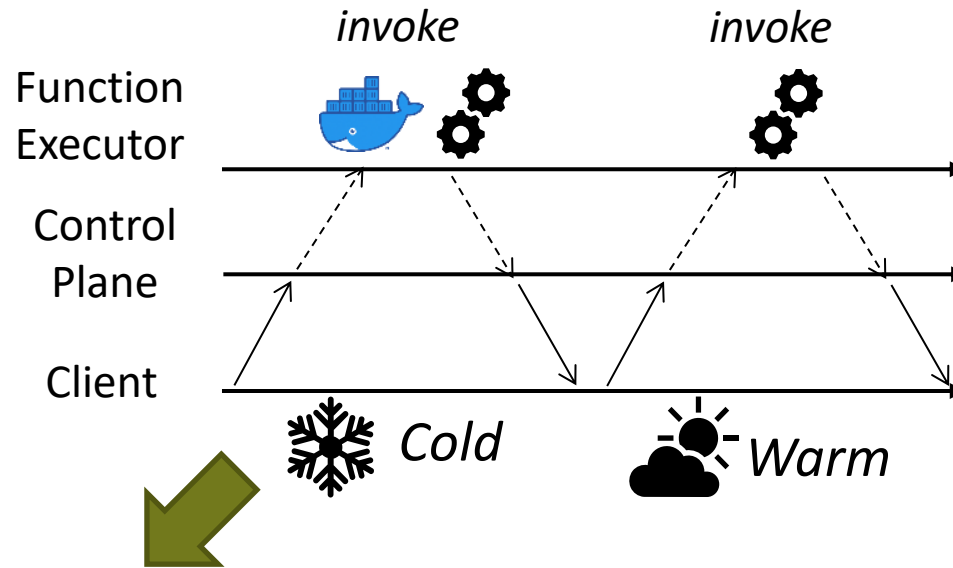
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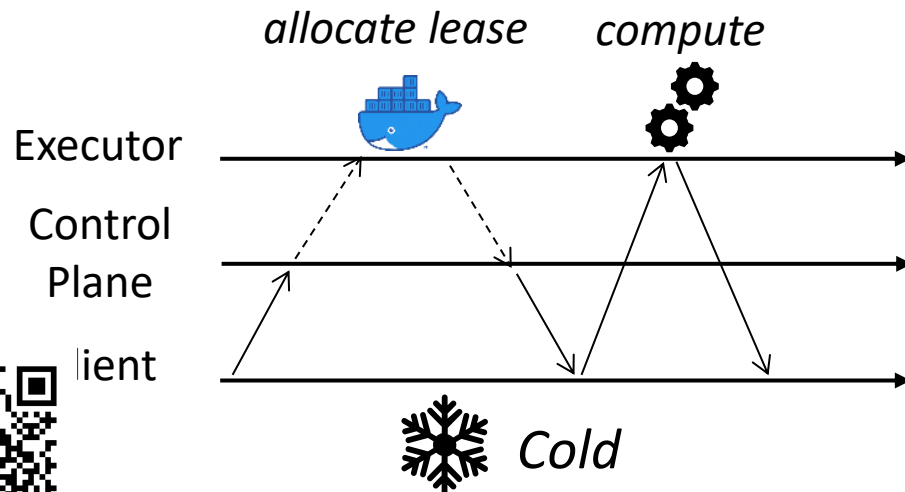
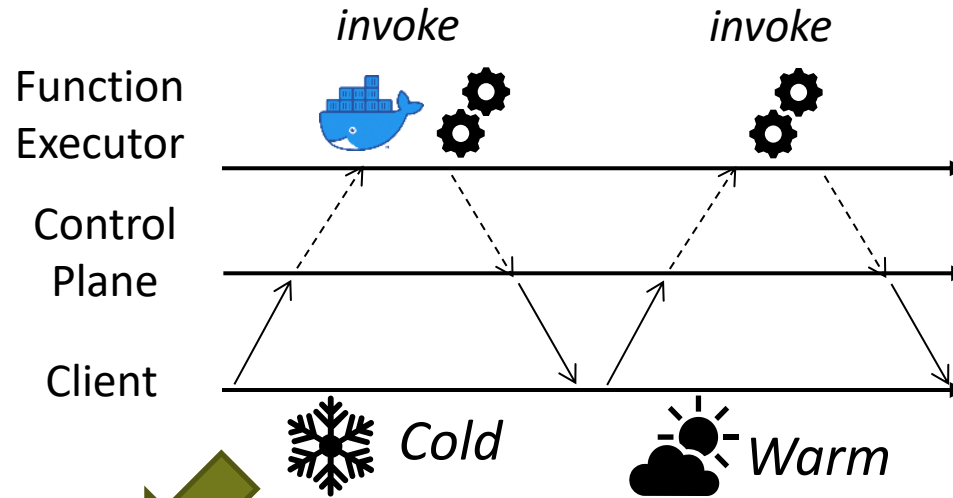
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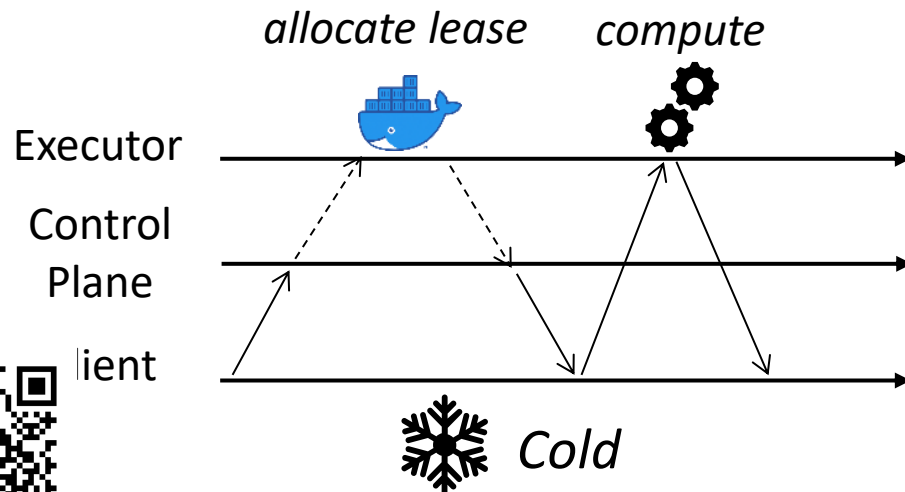
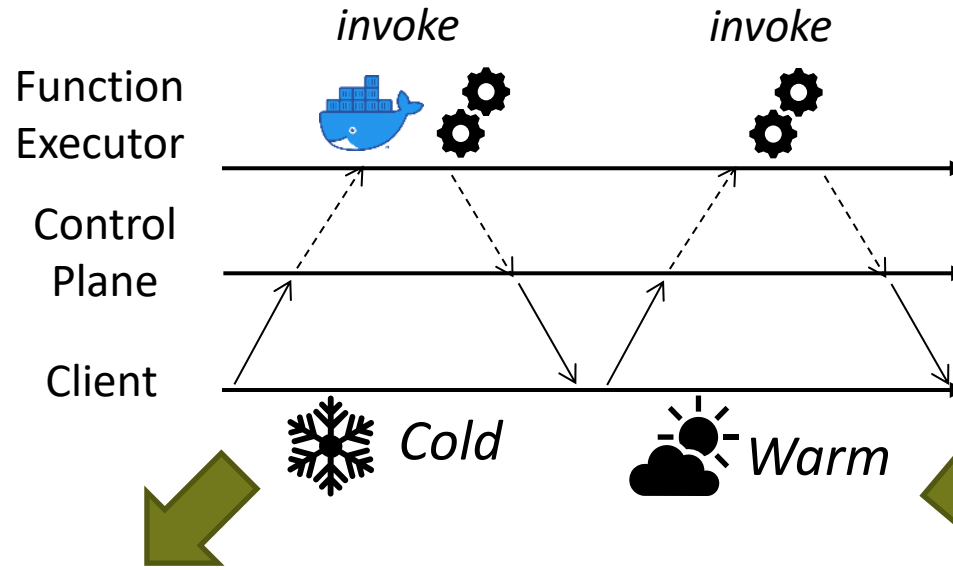
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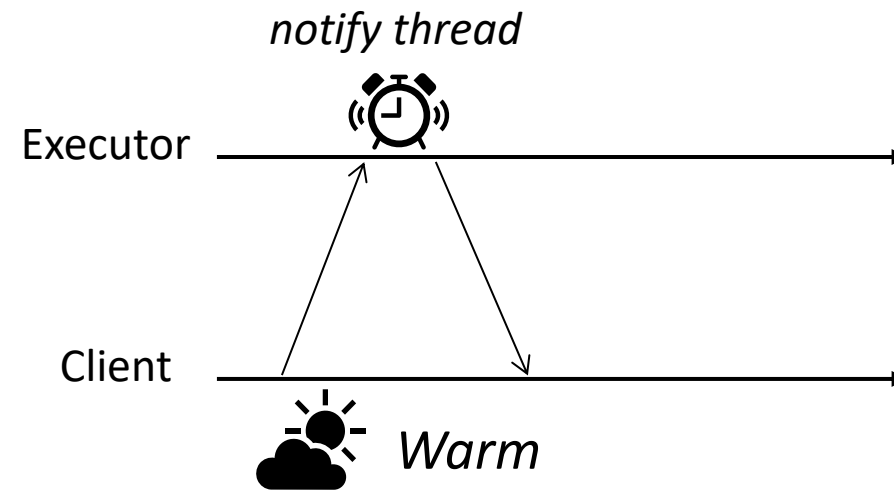
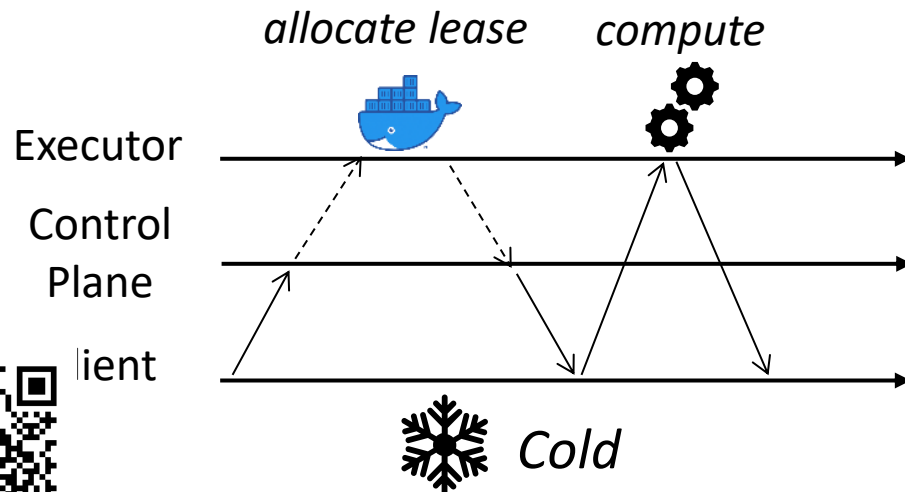
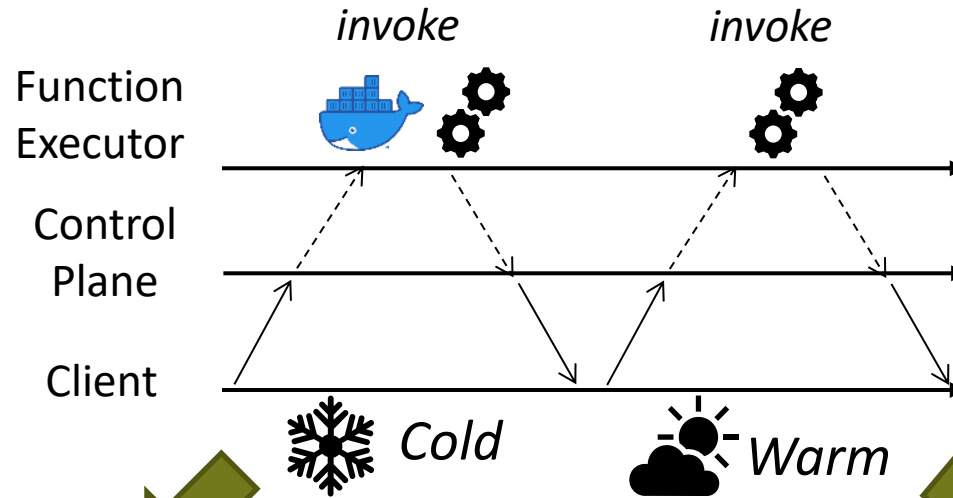
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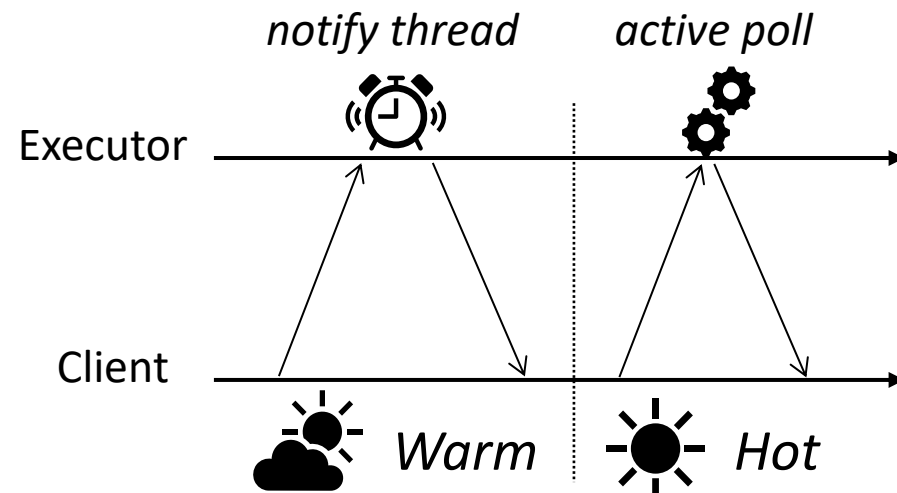
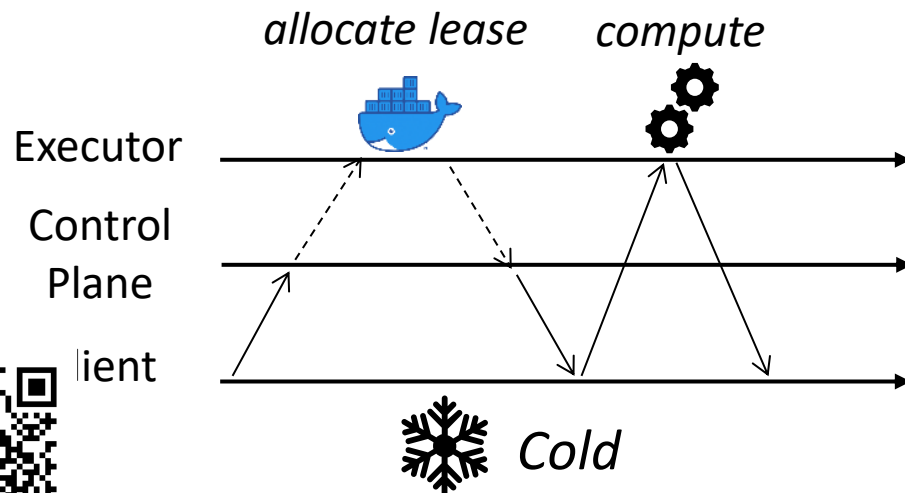
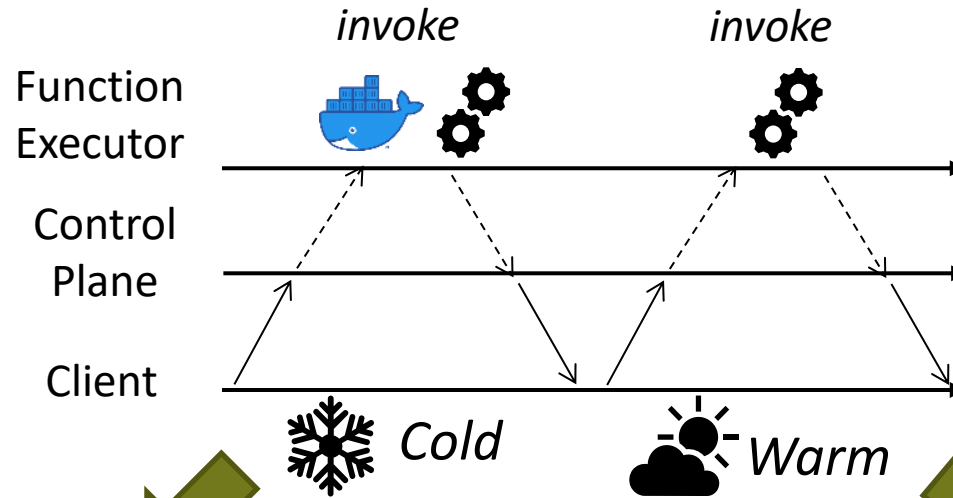
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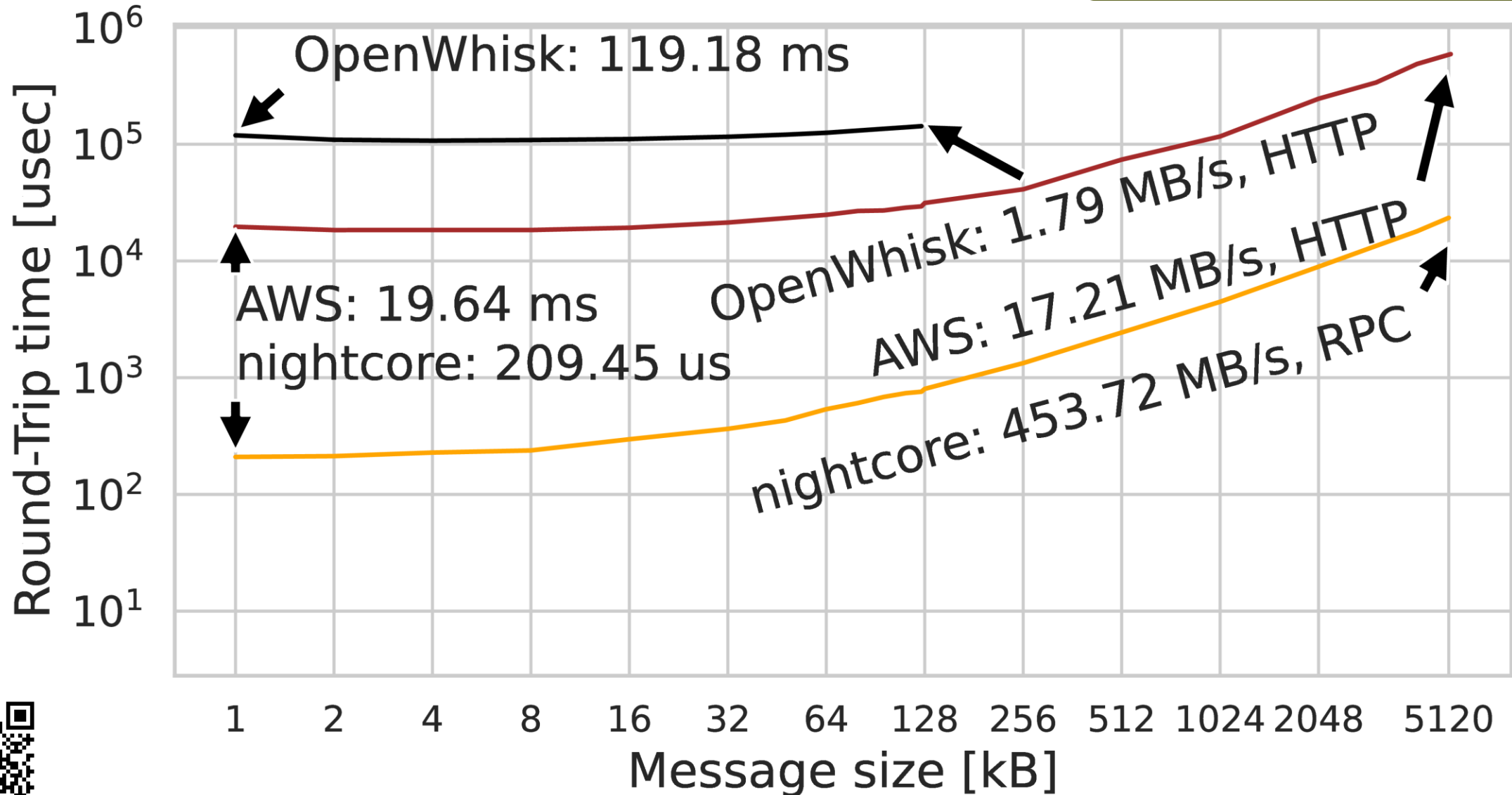


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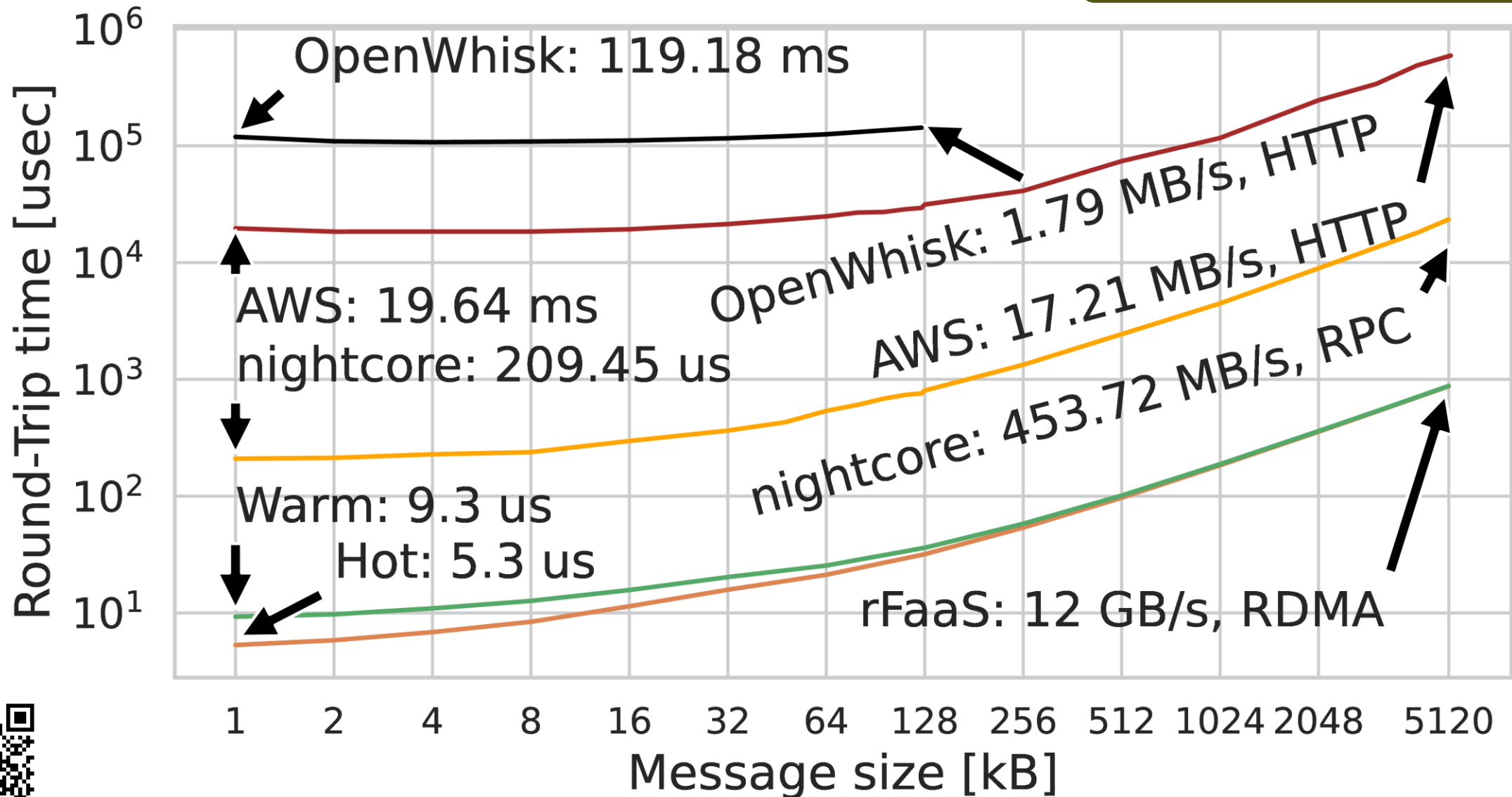
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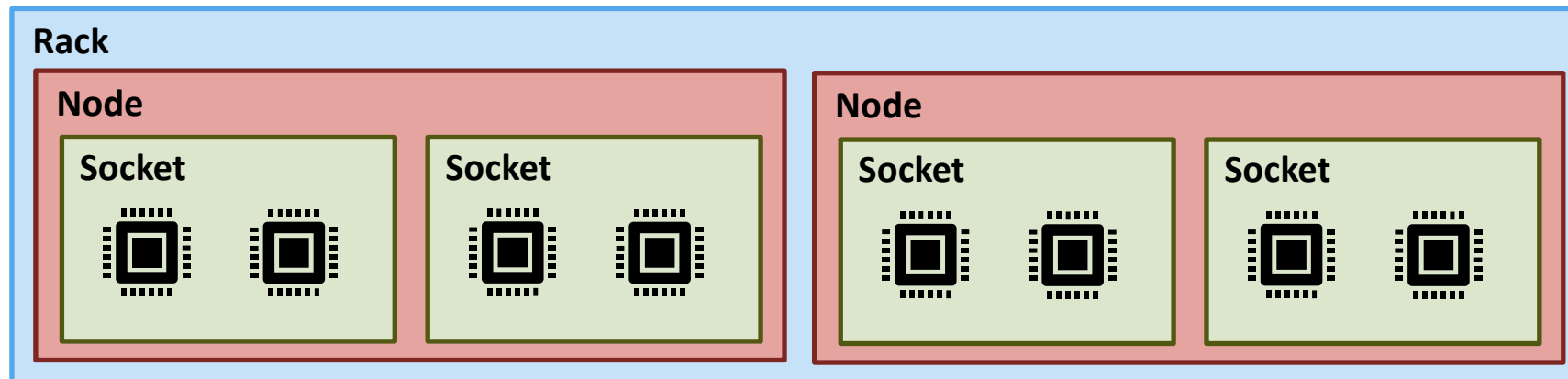
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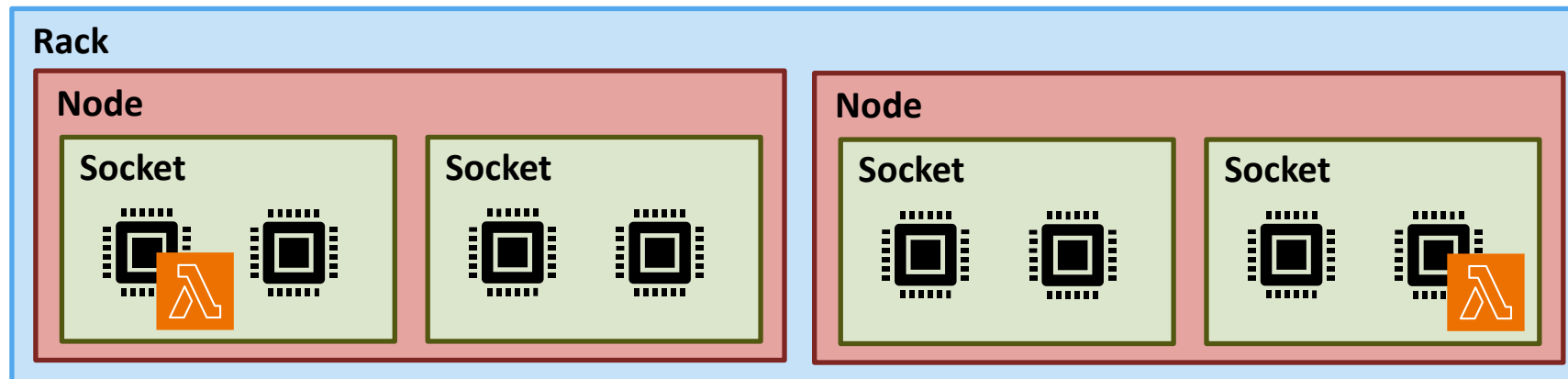
FMI: Serverless Communication

- ❖ We need **high performance**.
- ❖ We need **portable performance**.



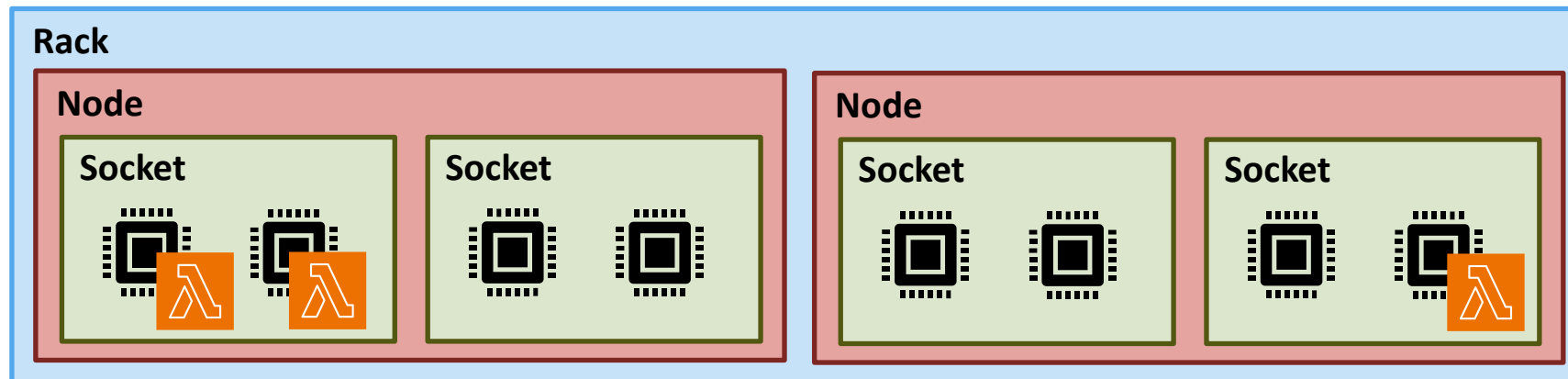
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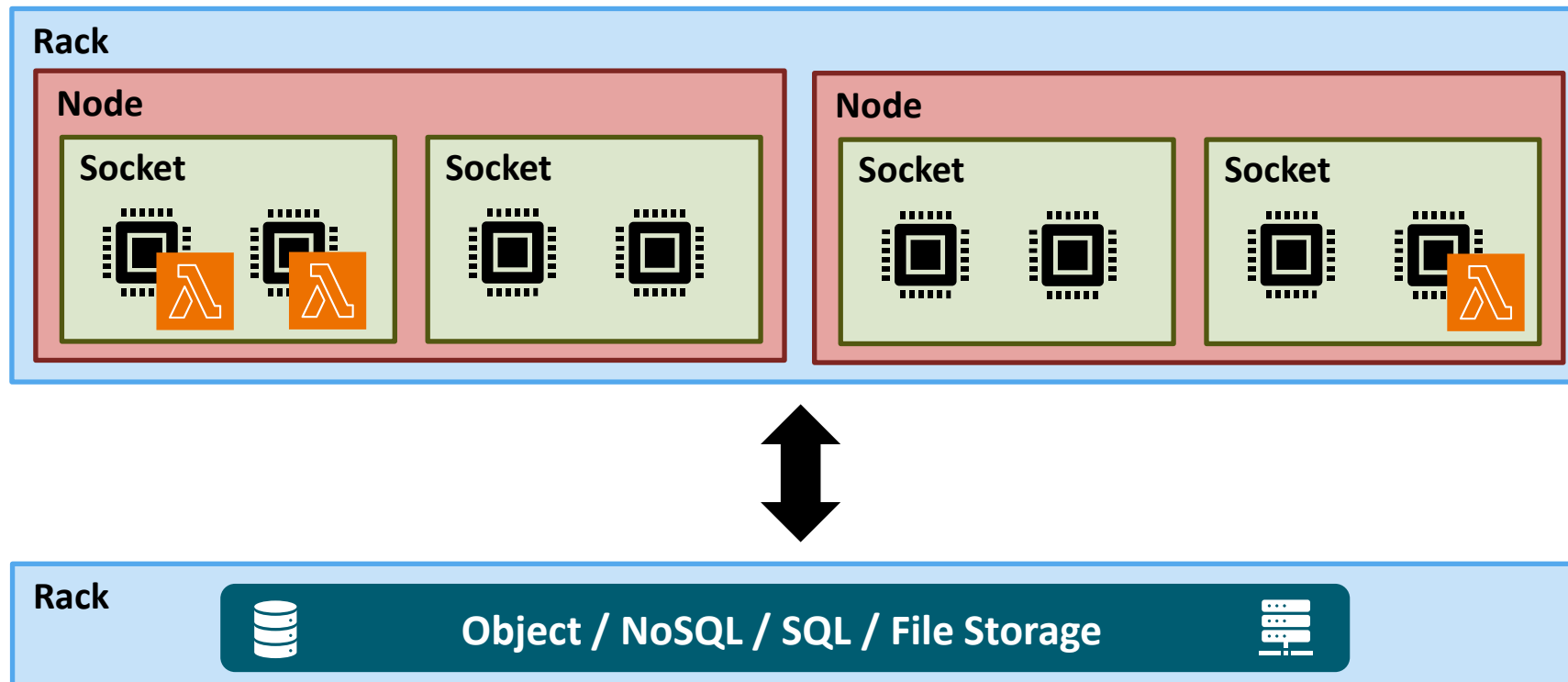
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FMI: Serverless Communication

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FMI: Slow Communication in Serverless

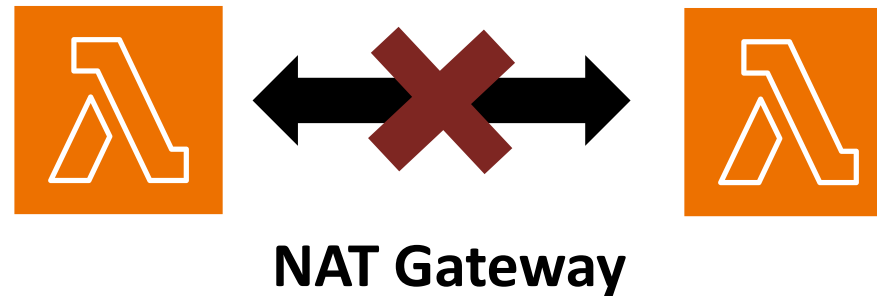


“FMI: Fast and Cheap Message Passing for Serverless Functions”, ICS’23

FMI: Slow Communication in Serverless

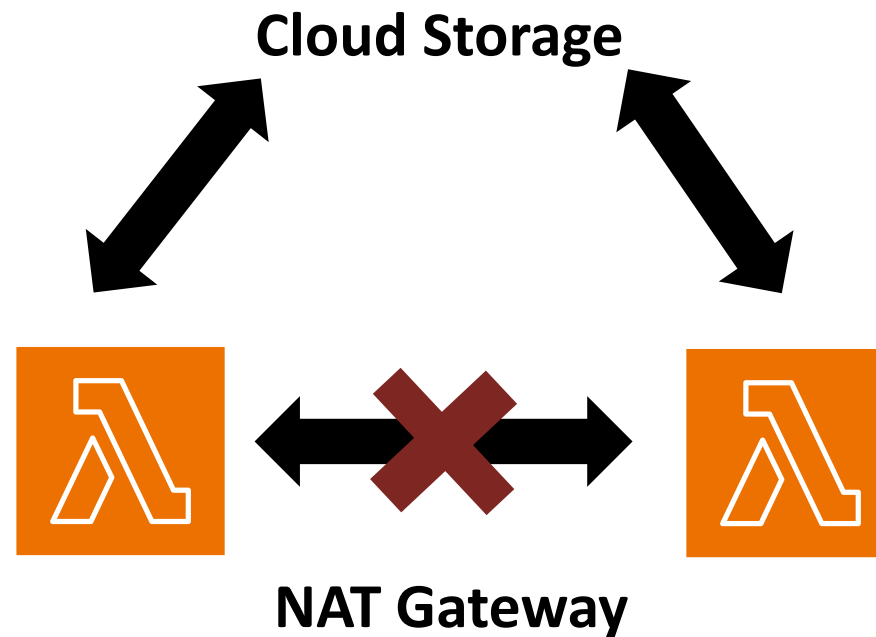


FMI: Slow Communication in Serverless



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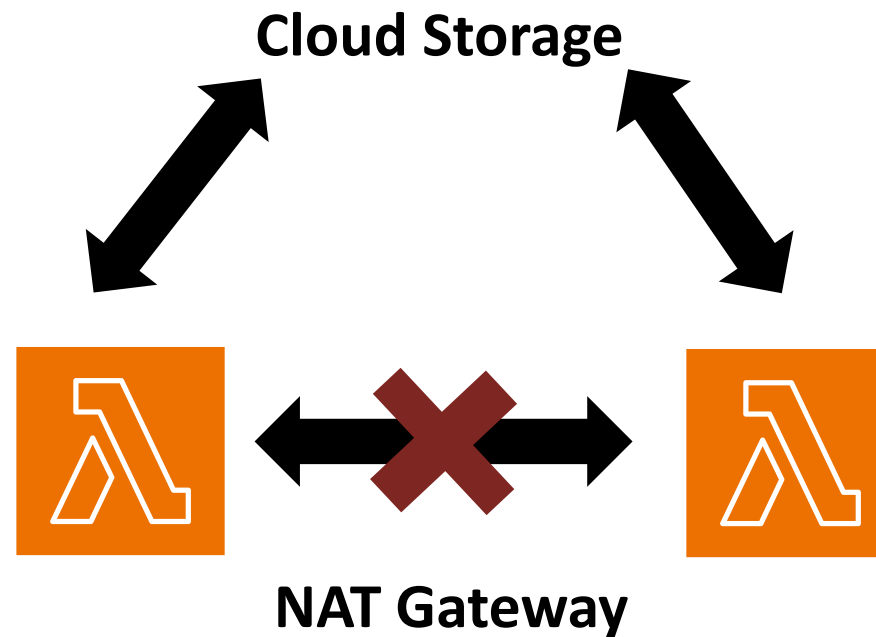


FMI: Slow Communication in Serverless

High Latency
For Small Messages



S3



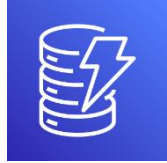
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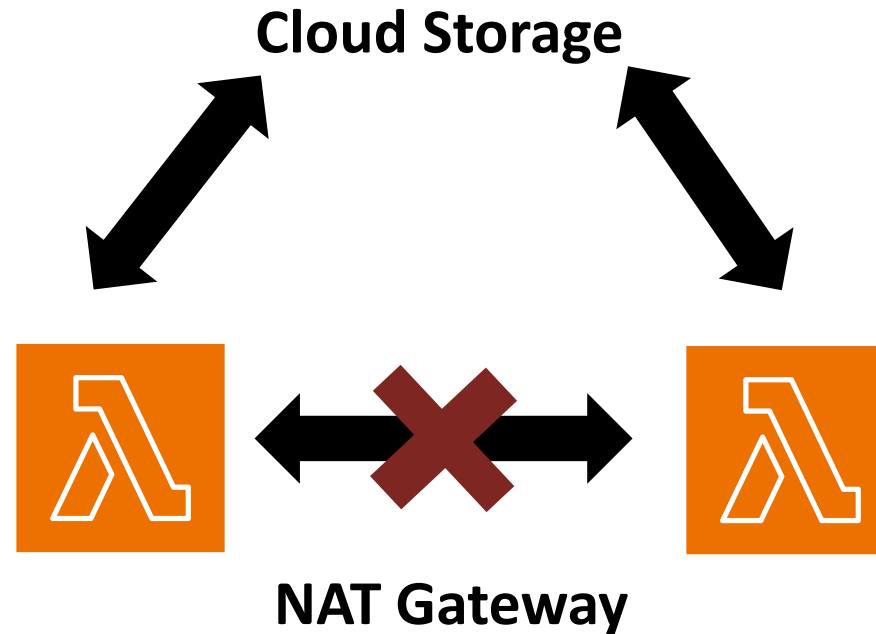


S3

Expensive for
Large Messages



DynamoDB



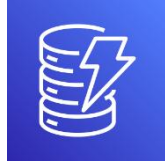
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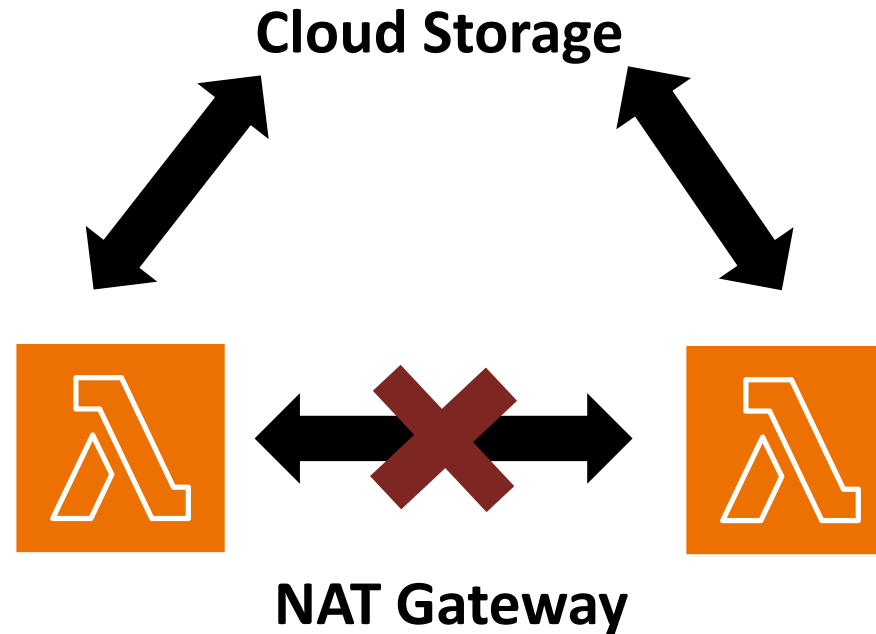


DynamoDB

Not Serverless
Expensive



Redis



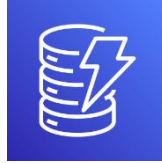
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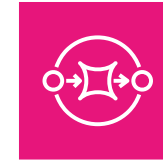
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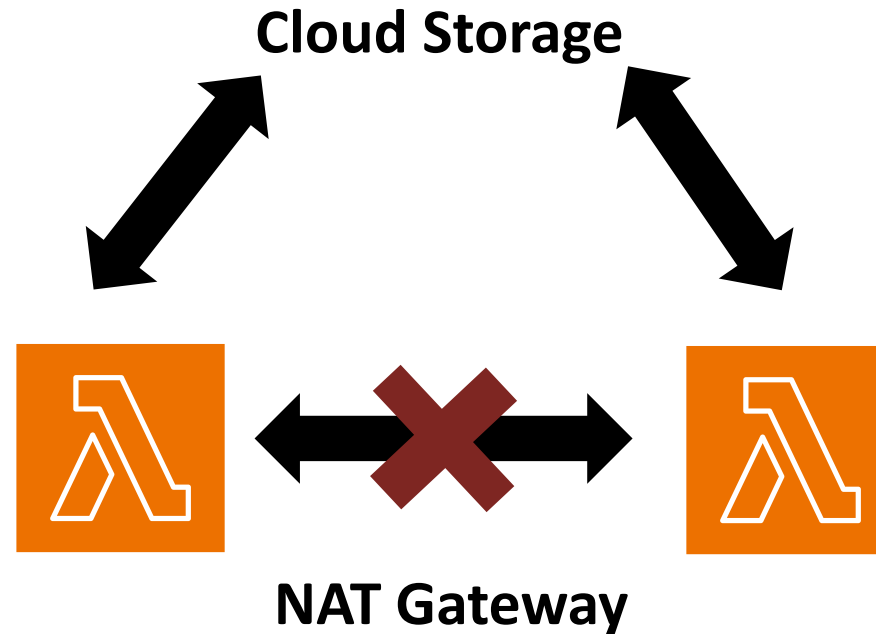


Redis

Size Limits
Good Latency



SQS



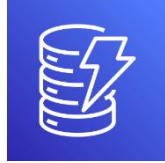
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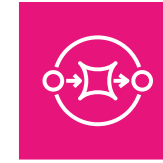
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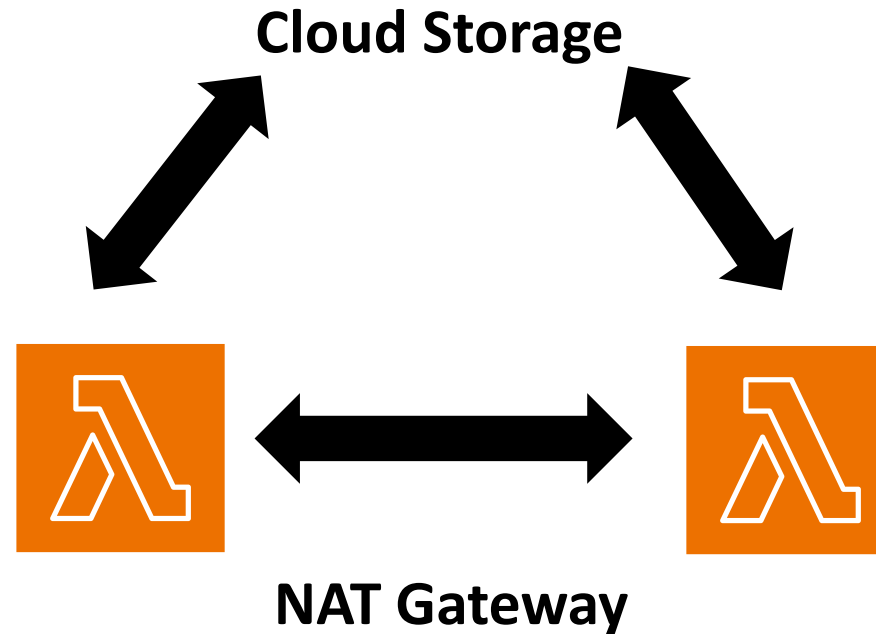


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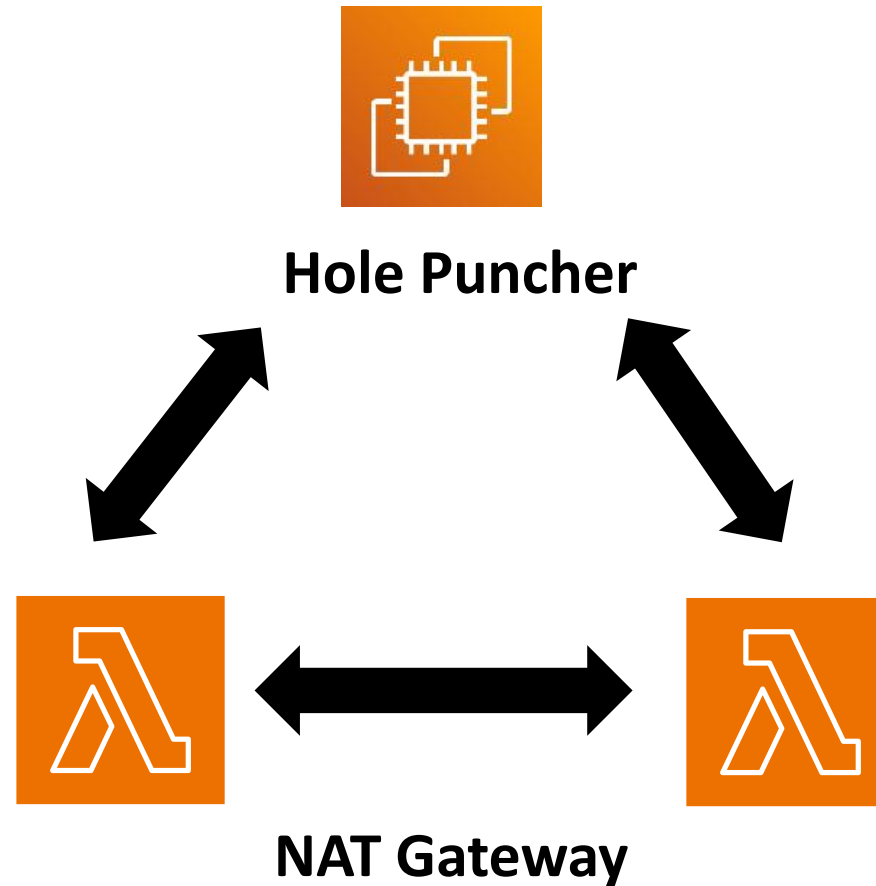
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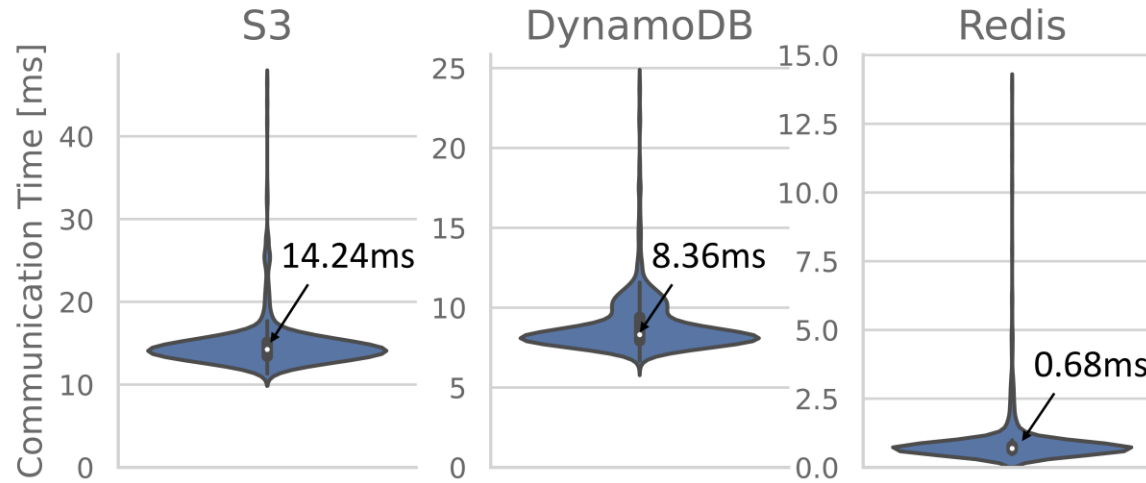
FMI: Fast Communication in Serverless



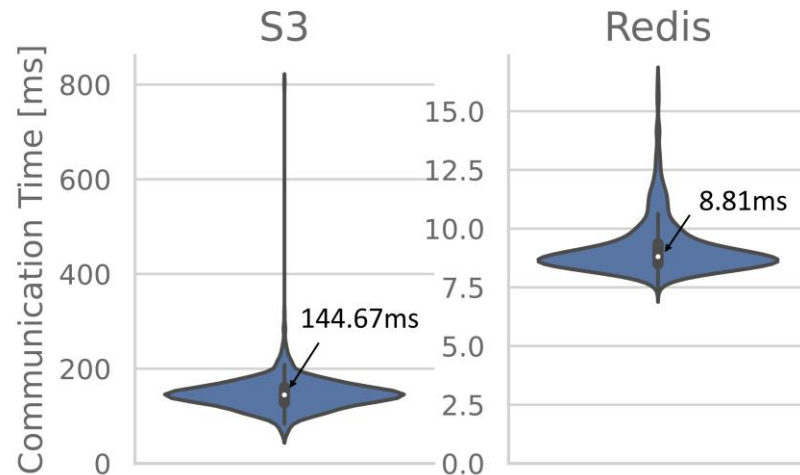
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Serverless Applications: Communication

1 B

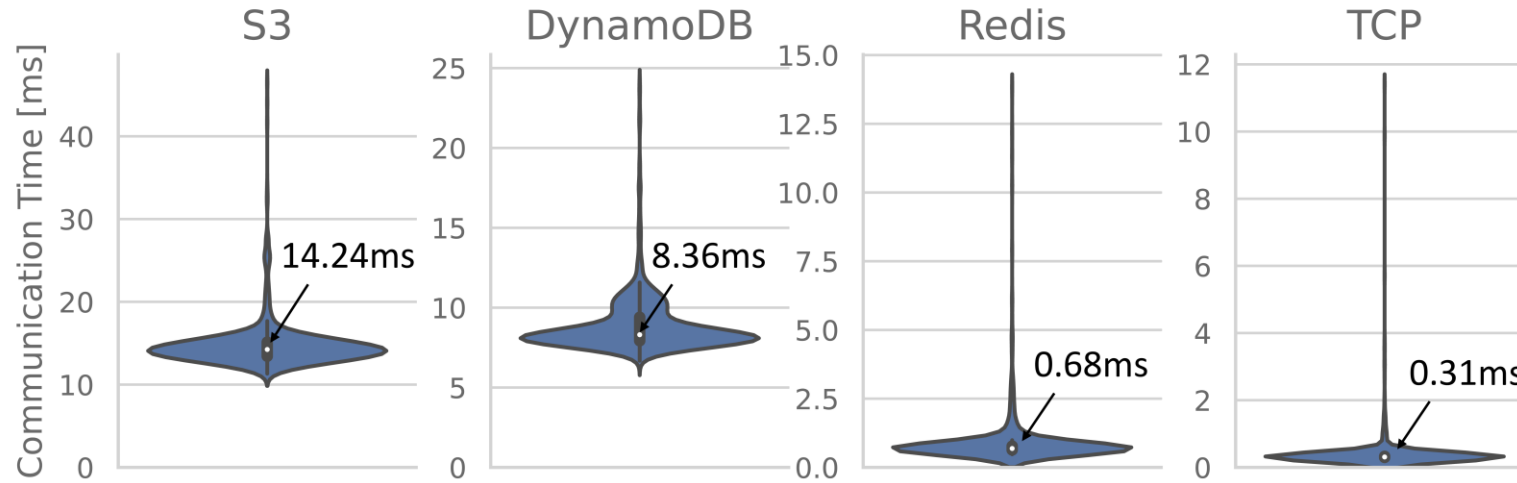


1 MB

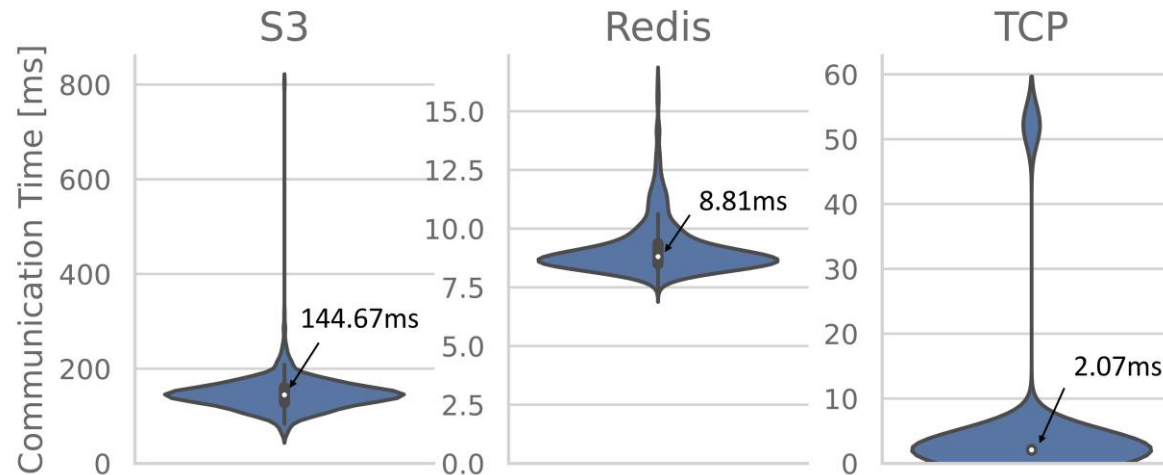


Serverless Applications: Communication

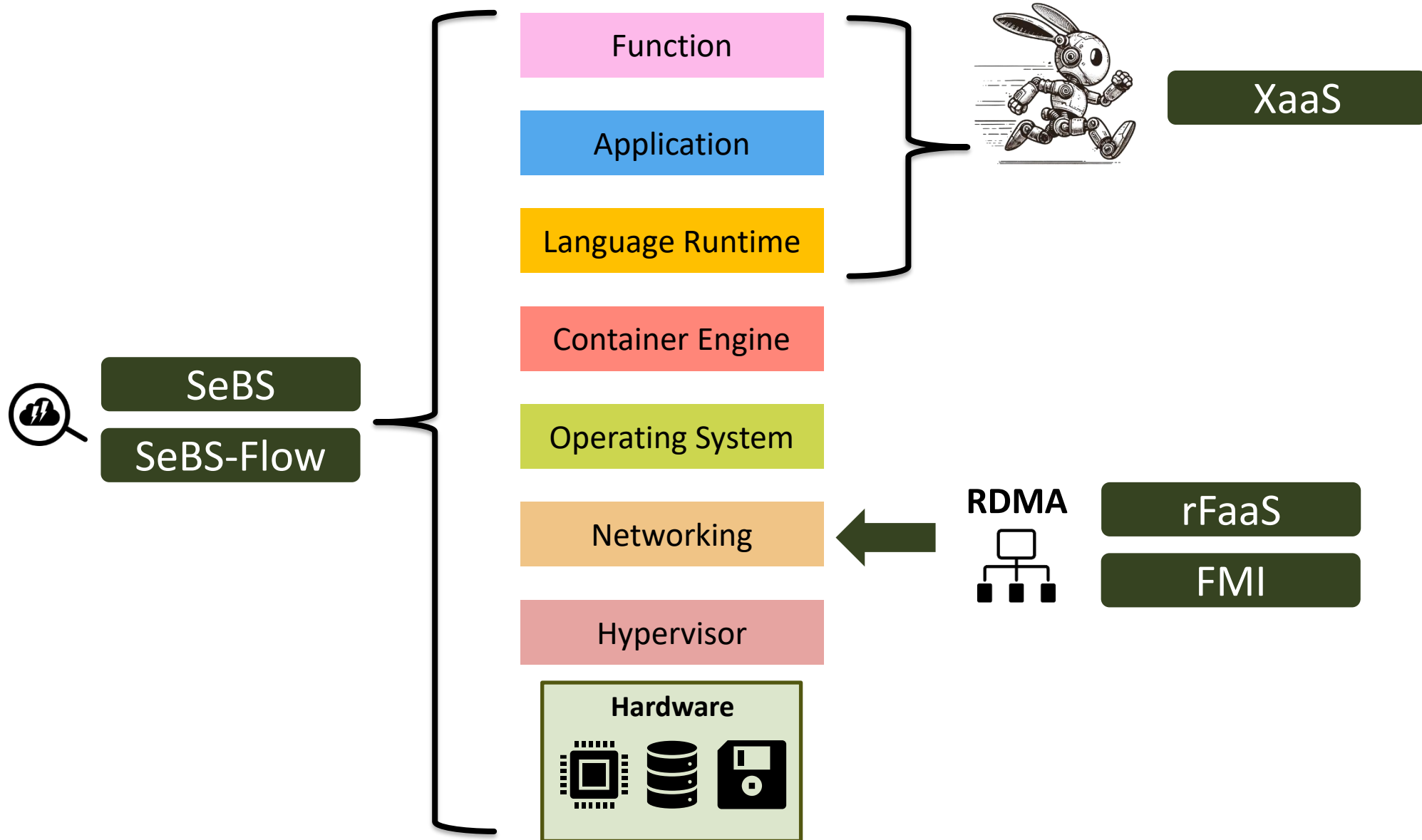
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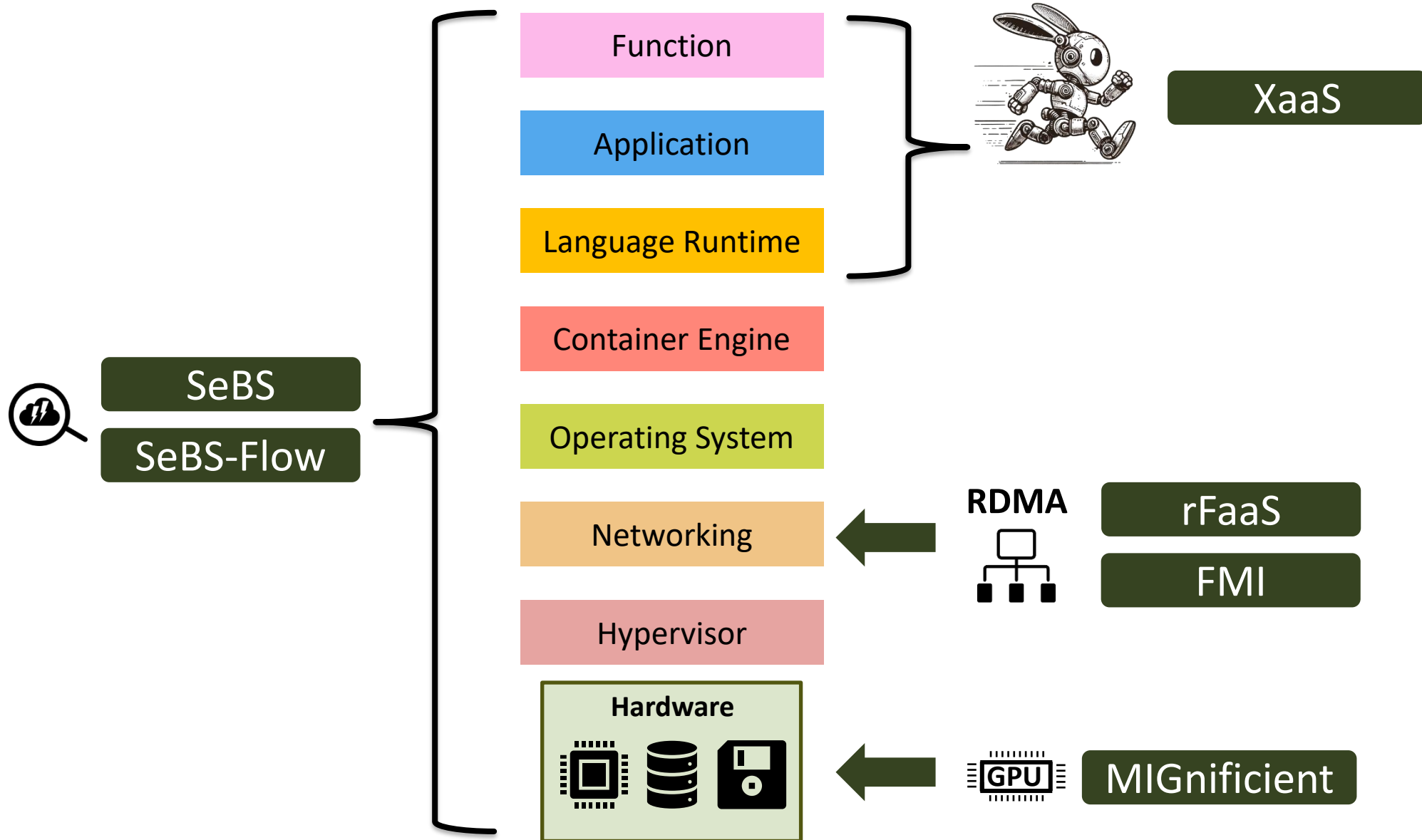
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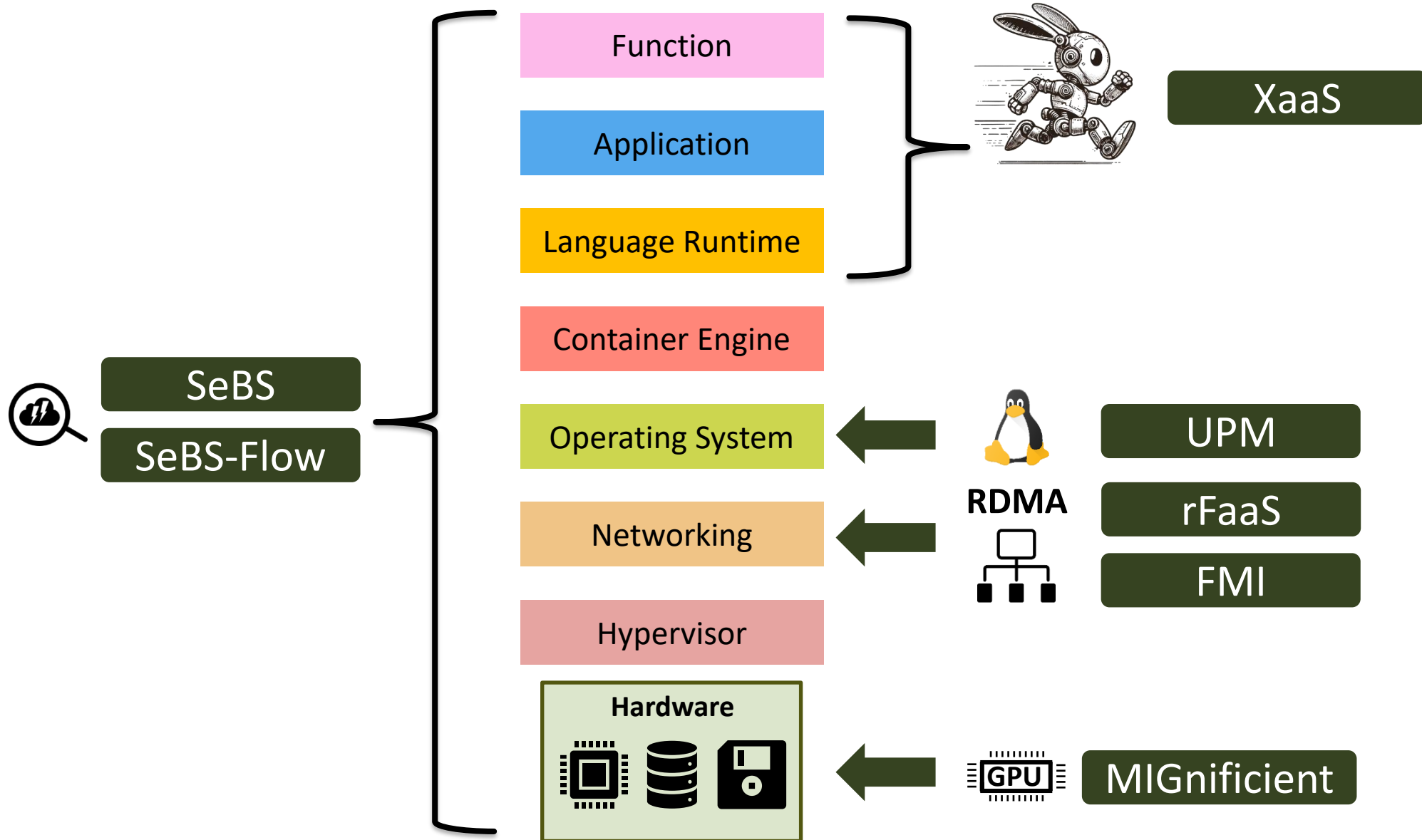
AXelerating Serverless Computing



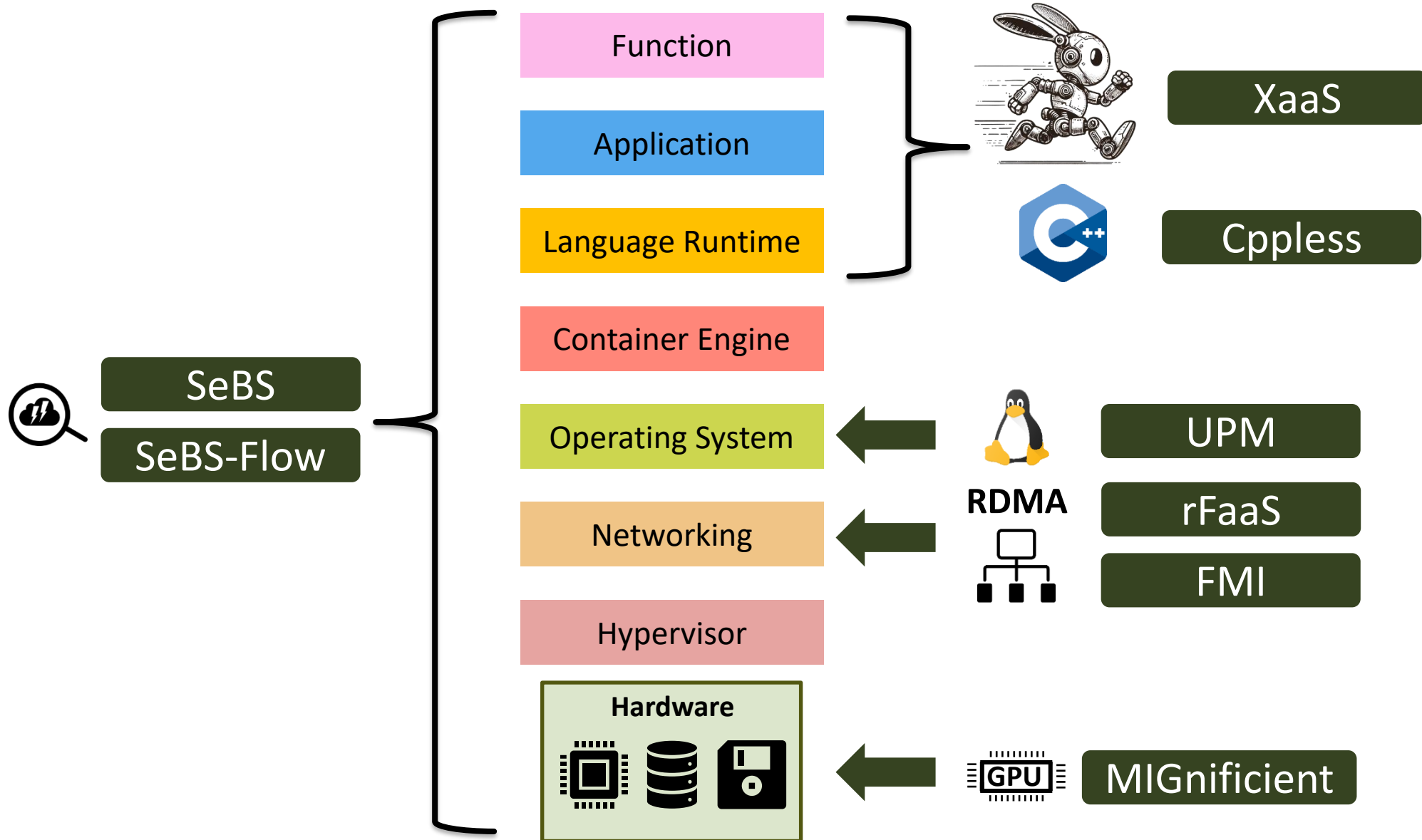
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AXelerating Serverless Computing



Let's deploy C++ on AWS Lambda!

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#include <aws/lambda-runtime/runtime.h>
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    using namespace Aws::Utils::Json;
    JsonValue json(request.payload);
    if (!json.WasParseSuccessful()) {
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(Cross) Compile to shared library.



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Link with custom runtime.



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Link with custom runtime.



Upload to cloud with all dependencies.

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(Cross) Compile to shared library.



Link with custom runtime.



Upload to cloud with all dependencies.

Let's deploy C++ on AWS Lambda!

```

#i
#i
#i
us
)
in
{
    Aws::Lambda::Model::InvokeRequest invokeRequest;
    invokeRequest.SetFunctionName(functionName);
    invokeRequest.SetInvocationType(
    Aws::Lambda::Model::InvocationType::RequestResponse);

    std::shared_ptr<Aws::IOStream> payload
        = Aws::MakeShared<Aws::StringStream>();
    Aws::Utils::Json::JsonValue jsonPayload;
    jsonPayload.WithInt64("iterations", iterations);
    *payload <<< jsonPayload.View().WriteReadable();
    invokeRequest.SetBody(payload);
    invokeRequest.SetContentType("application/json");

    ...
}
}
    
```

(Cross) Compile to shared library.



Link with custom runtime.

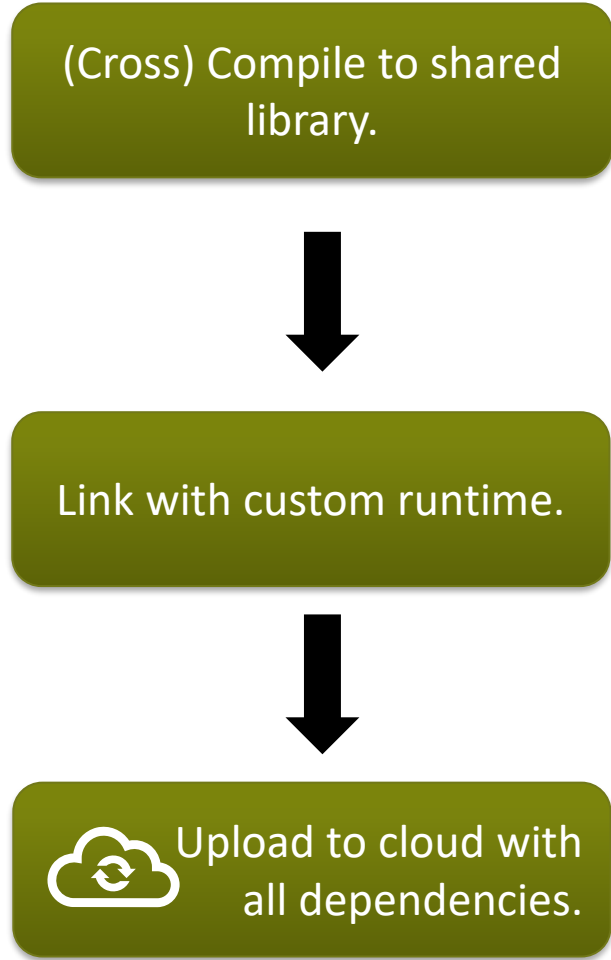


Upload to cloud with all dependencies.

Let's deploy C++ on AWS Lambda!

```

#include <string>
#include <string_view>
#include <memory>
...
using namespace Aws;
int main(int argc, char* argv[]) {
    {
        if (outcome.IsSuccess()) {
            auto &result = outcome.GetResult();
            Aws::IOStream &payload = result.GetPayload();
            Aws::String functionResult;
            std::getline(payload, functionResult);
            result = std::stoi(functionResult);
            return true;
        } else {
            return false;
        }
    }
    ...
}
    
```



Let's deploy C++ on AWS Lambda!

```

# Aws::SDKOptions options;
# Aws::InitAPI(options);
# Aws::Client::ClientConfiguration clientConfig;
auto m_client = Aws::MakeShared<Aws::Lambda::LambdaClient>(
    ALLOCATION_TAG,
    clientConfig
);
i
{
    int n = 10000;
    int np = 10;
    std::vector<int> results(np);
    std::vector<std::thread> threads;
    for (int i = 0; i < np; i++) {
        threads.emplace_back([&, i]() {
            InvokeFunction("pi-mc-worker", n / np, results[i]);
        });
    }

    for (auto &thread : threads) {
        thread.join();
    }
    auto pi = std::reduce(results.begin(), results.end()) / np;
}
  
```

(Cross) Compile to shared library.



Link with custom runtime.



Upload to cloud with all dependencies.

Challenges of C++ in Serverless

Challenges of C++ in Serverless

Complex, multi-source
project setup

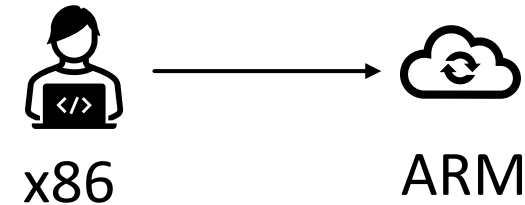
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for(int i = 0; i < n; ++i)  
    pi_mc(i);
```

Challenges of C++ in Serverless

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Cross-compiled environments

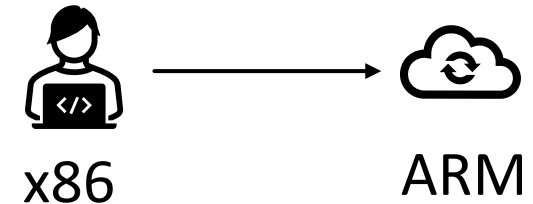


Challenges of C++ in Serverless

Complex, multi-source project setup

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```

Cross-compiled environments



Lack of static typing



Manual verification?
JSON Schema?

Cppless: Single-source C++ Compiler for Serverless

```
double pi_mc(int n);

double pi_estimate()
{
    const int n = 100000000;
    const int np = 128;

    cppless::aws_dispatcher dispatcher;
    auto aws = dispatcher.create_instance();

    std::vector<double> results(np);
    auto fn = [=] { return pi_mc(n / np); };

    for (auto& result : results)
        cppless::dispatch(aws, fn, result);
    cppless::wait(aws, np);

    auto pi = std::reduce(
        results.begin(), results.end()
    ) / np;

    return pi;
}
```



spcl/cppless

Cppless: Single-source C++ Compiler for Serverless

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```

```
double pi_estimate()
```

```
{
```

```
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```
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```

```
    return pi;
```

```
}
```



C++ abstraction for cloud provider APIs.

Avoids the vendor lock-in and simplifies invocations.



spcl/cppless

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{
    const int n = 100000000;
    const int np = 128;

    cppless::aws_dispatcher dispatcher;
    auto aws = dispatcher.create_instance();

    std::vector<double> results(np);
    auto fn = [=] { return pi_mc(n / np); };

    for (auto& result : results)
        cppless::dispatch(aws, fn, result);
    cppless::wait(aws, np);

    auto pi = std::reduce(
        results.begin(), results.end()
    ) / np;

    return pi;
}
```



C++ abstraction for cloud provider APIs.

Avoids the vendor lock-in and simplifies invocations.



Serverless function as C++ lambda expression.

Automatically compiled to a cloud function.



spcl/cppless

Cppless: Single-source C++ Compiler for Serverless

```
double pi_mc(int n);
```

```
double pi_estimate()
```

```
{
```

```
    const int n = 100000000;
```

```
    const int np = 128;
```

```
    cppless::aws_dispatcher dispatcher;  
    auto aws = dispatcher.create_instance();
```

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    std::vector<double> results(np);  
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```
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```
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```



C++ abstraction for cloud provider APIs.

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Serverless function as C++ lambda expression.

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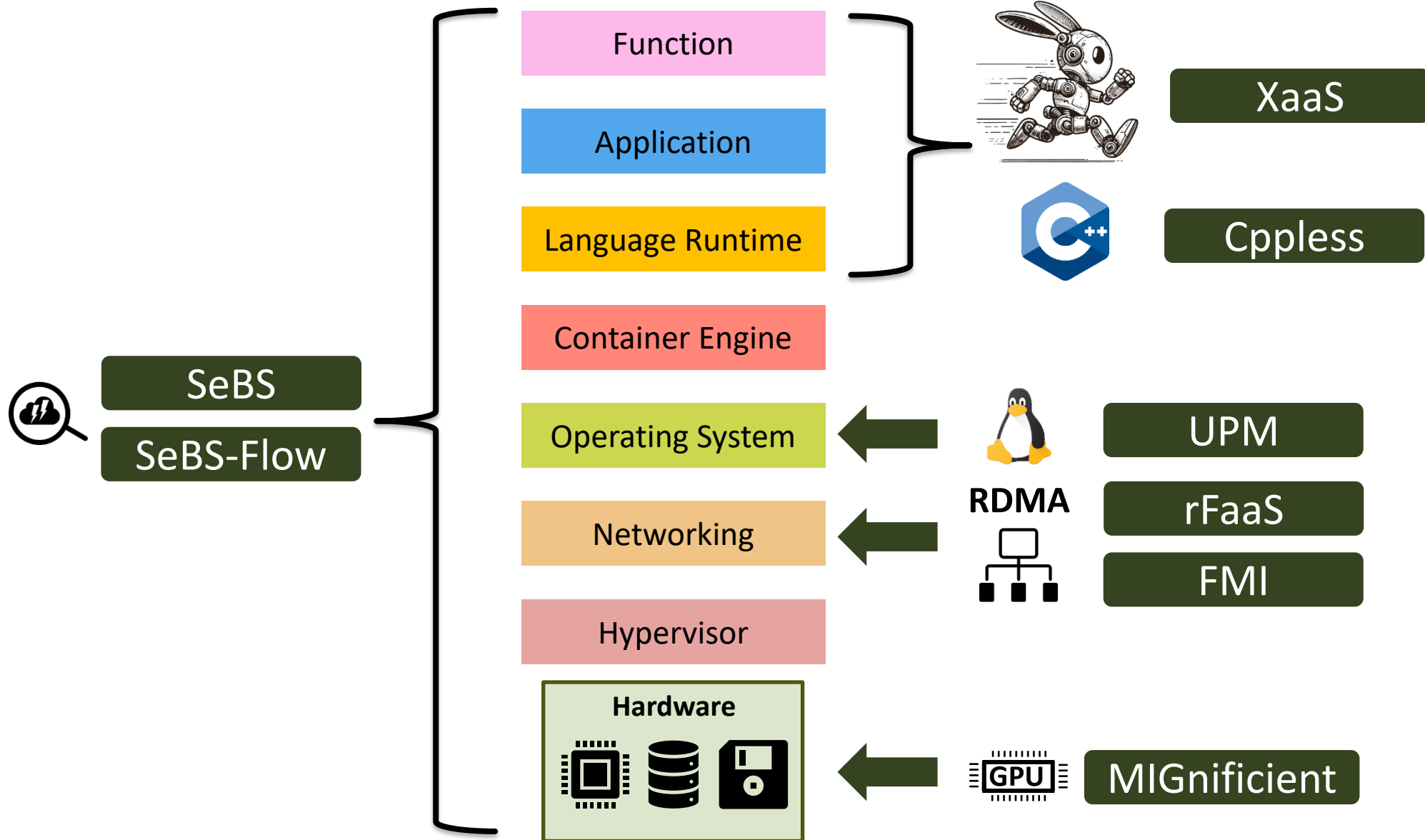
Integrated invocation of the function.

Automatic serialization and type checking.

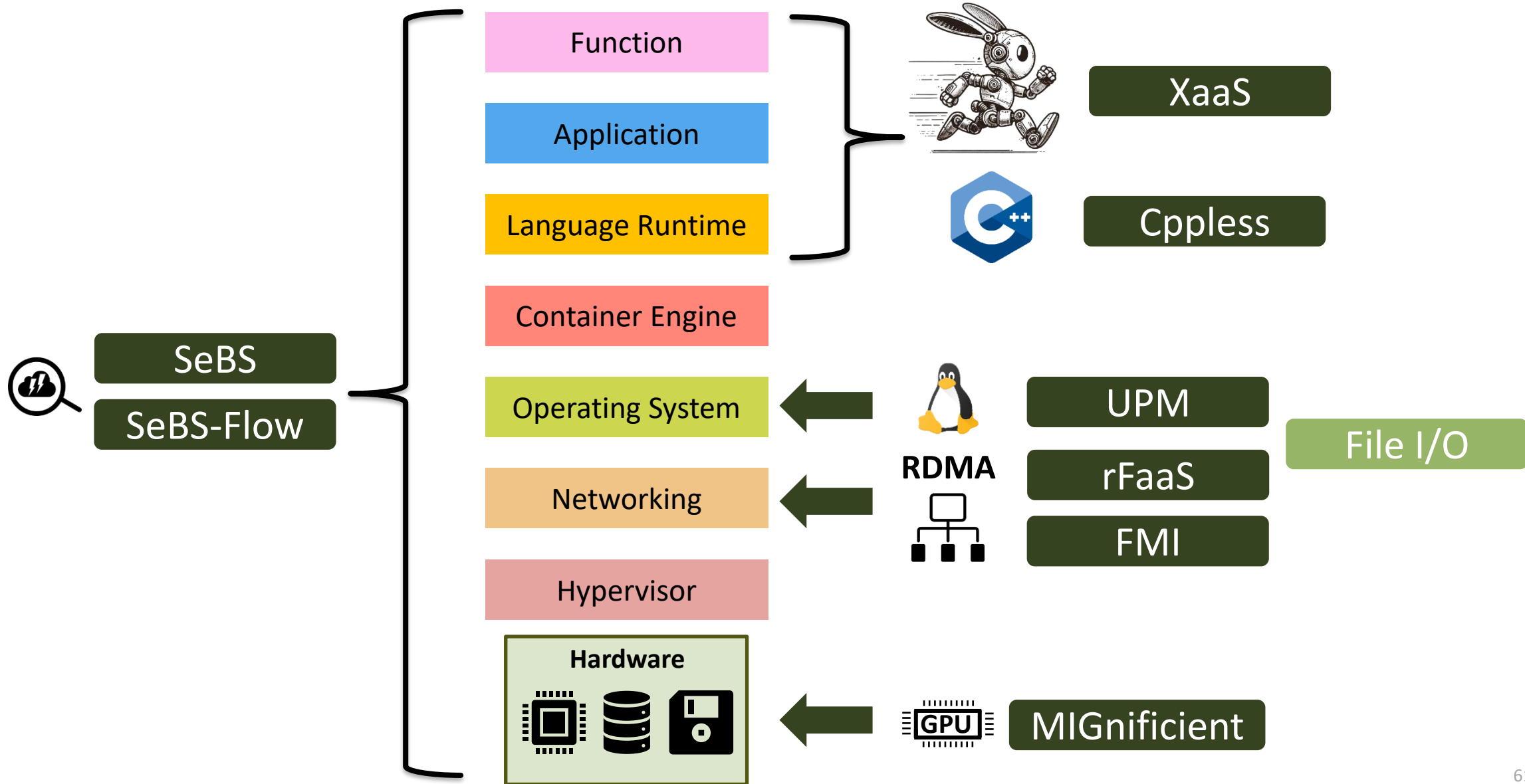


spcl/cppless

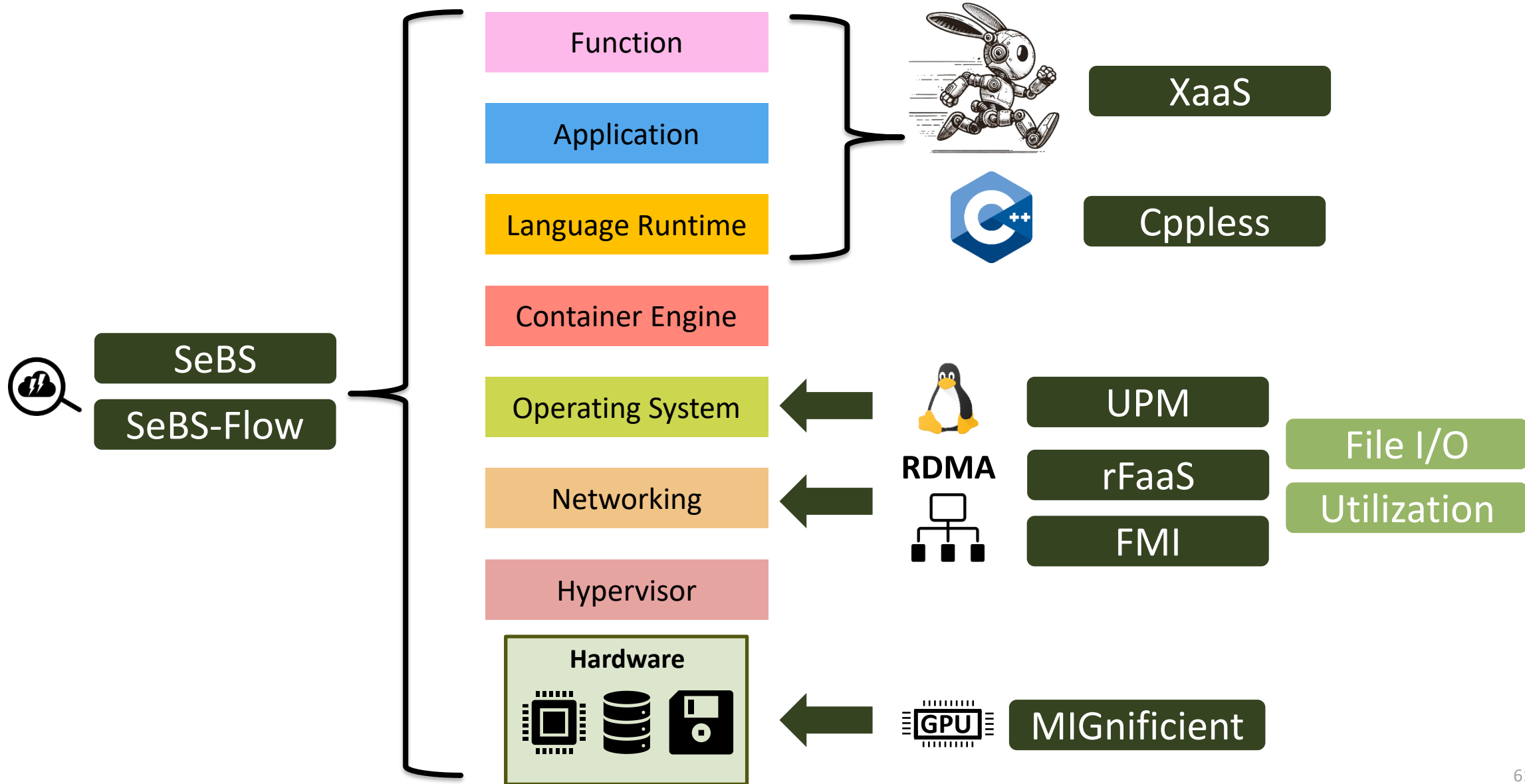
AXelerating Serverless Computing: Ongoing Work & Future



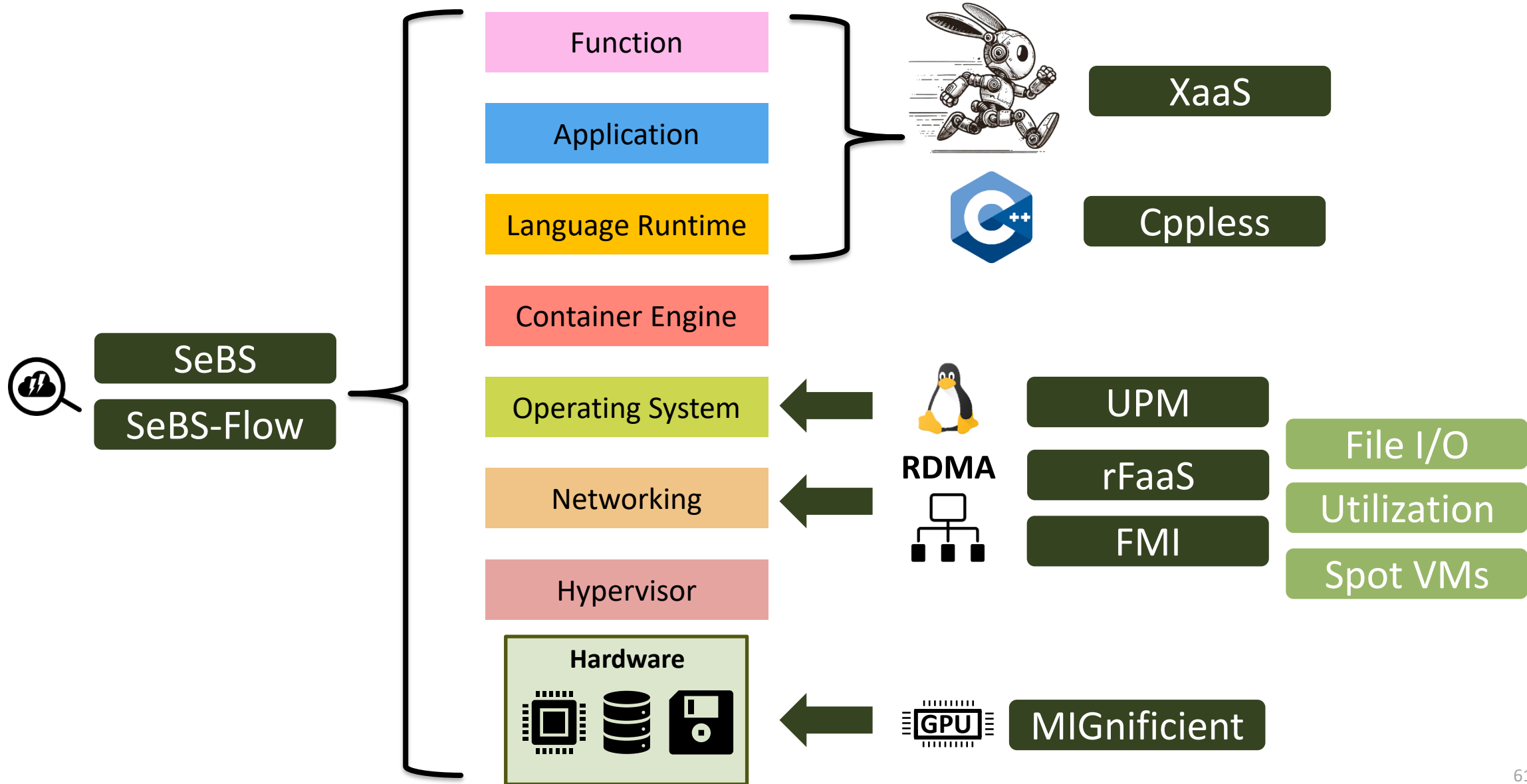
AXelerating Serverless Computing: Ongoing Work & Future



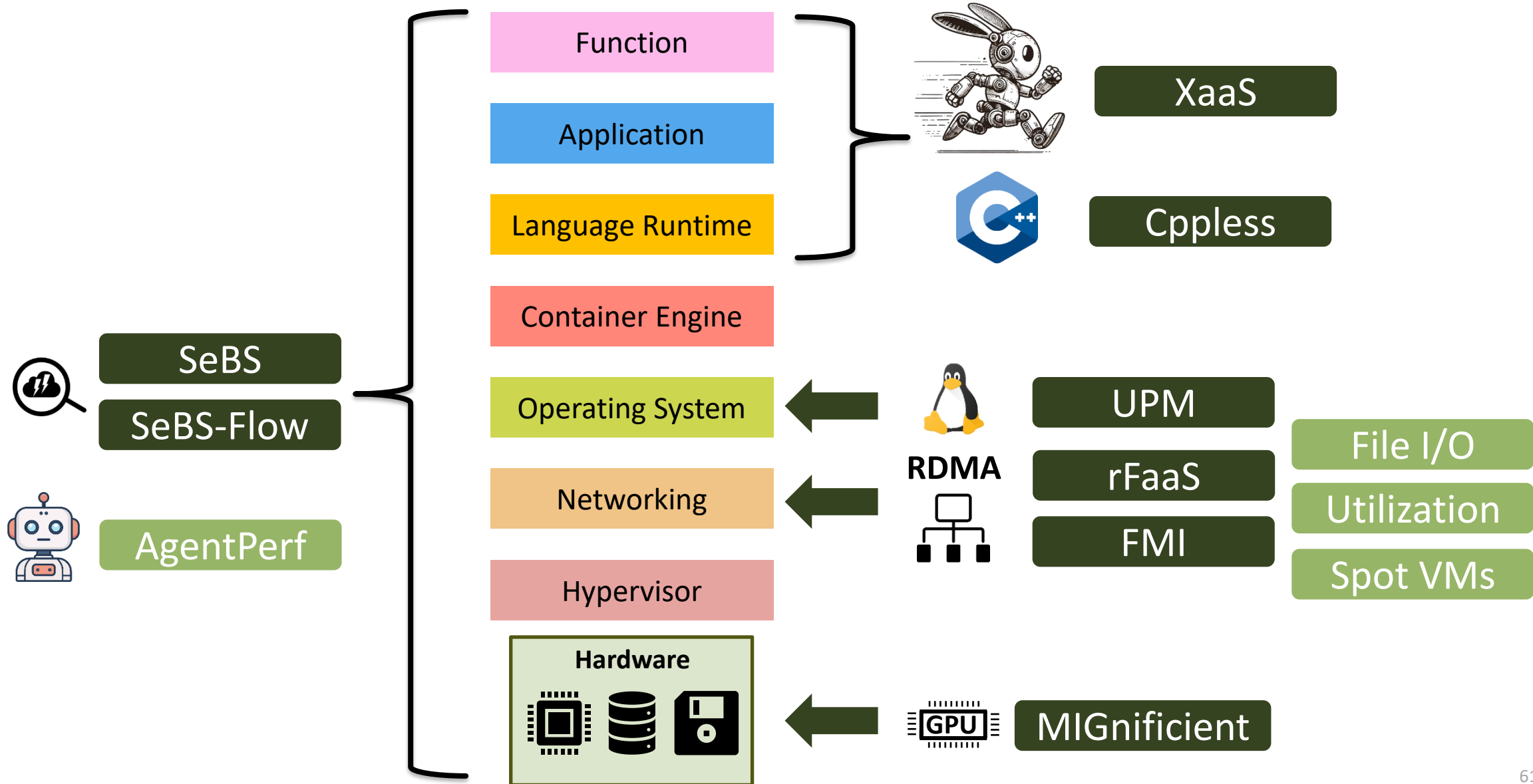
AXelerating Serverless Computing: Ongoing Work & Future



AXelerating Serverless Computing: Ongoing Work & Future





AXelerating Serverless Computing: Ongoing Work & Future



High-Performance Solutions for Serverless

 **spcl/serverless-benchmarks**


 **spcl/rFaaS**

 **spcl/PraaS**

 **spcl/FaaSKeeper**

 **spcl/XaaS**

 **spcl/FMI**

 **spcl/cppless**

Conclusions

With contributions from: Alexandru Calotoiu, Torsten Hoefler, Maciej Besta, Laurin Brandner, Rodrigo Bruno, Roman Böhringer, Tiancheng Chen, Marcin Chrapek, Jakub Czerski, Nico Graf, Tobias Grosser, Laurin Jahns, Kacper Janda, Sascha Kehrli, Prajin Khadka, Mateusz Knapik, Abhishek Kumar, Grzegorz Kwaśniewski, Horia Mercan, Michał Podstawski, Wei Qiu, Gyorgy Rethy, Oana Rosca, Mahla Sarifi, Larissa Schmid, Konstantin Taranov, Nicolas Wicki, Felix Wolf, Yuejian Yu, Pengyu Zhou, Paweł Żuk,

More of SPCL's research:

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... or spcl.ethz.ch



Serverless HPC Projects




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Serverless HPC Projects



Research into Serverless Performance

Research into Serverless Performance



Fast and Lightweight Sandboxes
(gVisor, Catalyzer, SEUSS, Photon)

Research into Serverless Performance



Fast and Lightweight Sandboxes
(gVisor, Catalyzer, SEUSS, Photon)



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(Cloudburst, Faasm, Crucial, PraaS)

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HPC FaaS

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(Cirrus, LambdaML, Mashup, DayDream)



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HPC Utilization

(HPC-Whisk, Serverless Disaggregation)

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Benchmark Suites

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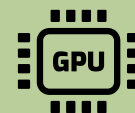
Improved Cold Starts

(RainbowCake, IceBreaker, Medes)



HPC Utilization

(HPC-Whisk, Serverless Disaggregation)



Accelerated Functions

(DGFS, KaaS, MIGnificent)

Serverless: One Step Toward HPC – Cloud Convergence

Infrastructure



Serverless: One Step Toward HPC – Cloud Convergence




Infrastructure



Serverless: One Step Toward HPC – Cloud Convergence

Infrastructure



-  Virtual Machines
-  Object Storage
-  Virtual Networks






HPCaaS



Serverless: One Step Toward HPC – Cloud Convergence

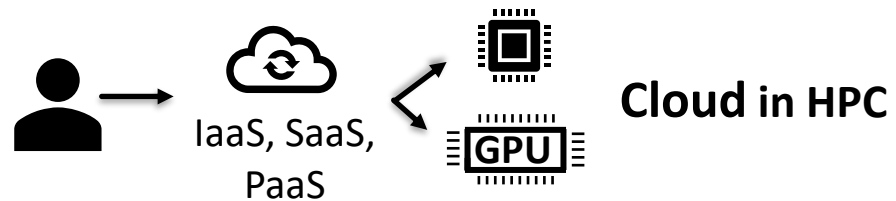
Infrastructure



-  Virtual Machines
-  Object Storage
-  Virtual Networks



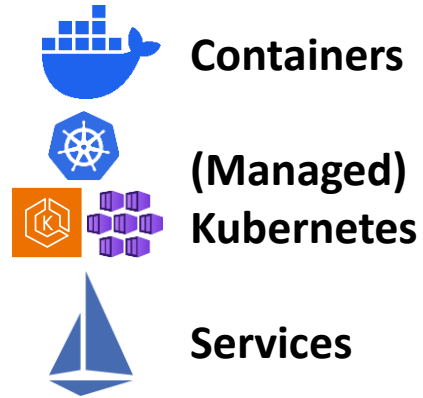
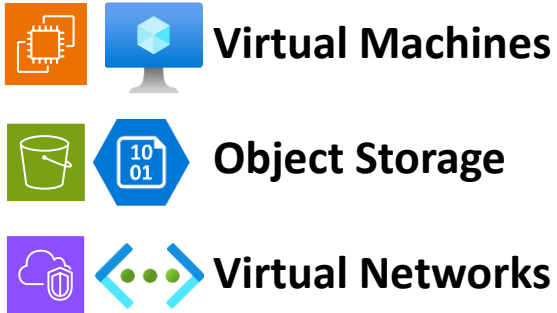
HPCaaS



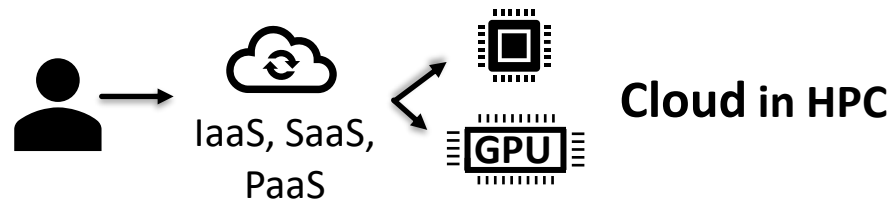
Serverless: One Step Toward HPC – Cloud Convergence

Infrastructure

Deployment



HPCaaS









Serverless: One Step Toward HPC – Cloud Convergence

Infrastructure

Deployment

Cloud

-  Virtual Machines
-  Object Storage
-  Virtual Networks

-  Containers
-  (Managed) Kubernetes
-  Services

HPC


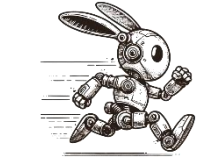
HPCaaS

-  HPC in the cloud
-  F u g a k u

-  SARUS
-  HPC
-  Containers

Cloud in HPC



-  Flux
-  XaaS

Serverless: One Step Toward HPC – Cloud Convergence

Infrastructure

Deployment

Compute



- Virtual Machines
- Object Storage
- Virtual Networks

- Containers
- (Managed) Kubernetes
- Services

- Serverless Functions
- Serverless Containers



HPCaaS

- HPC in the cloud
- Fugaku

- SARUS
- HPC
- Containers

Flux

XaaS

Cloud in HPC



Serverless: One Step Toward HPC – Cloud Convergence

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HPCaaS

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- Fugaku

- SARUS
- HPC Containers

- Globus Compute (funcX)

- Flux

- RDMA rFaaS

- XaaS

- Lithops



Serverless: One Step Toward HPC – Cloud Convergence

Infrastructure

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Applications



- Virtual Machines
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- Virtual Networks

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- Serverless Containers

- Dask, Spark Ray
- Serverless Workflows



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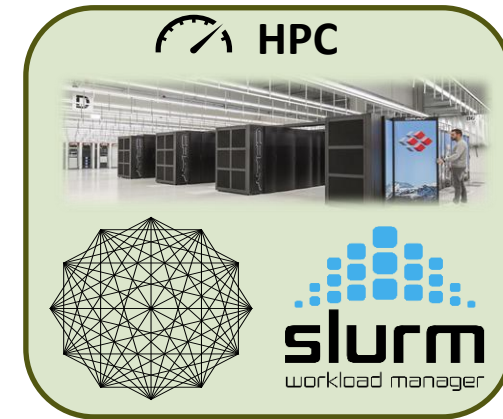
- XaaS

- Lithops

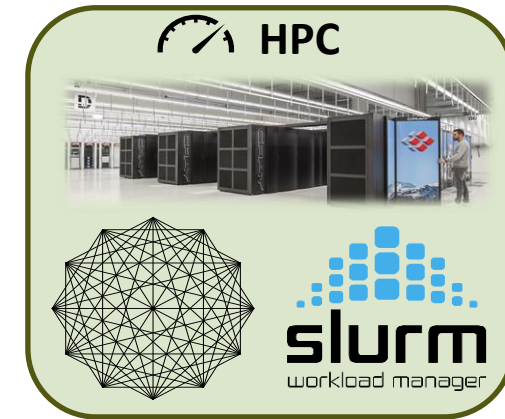


Cloud in HPC

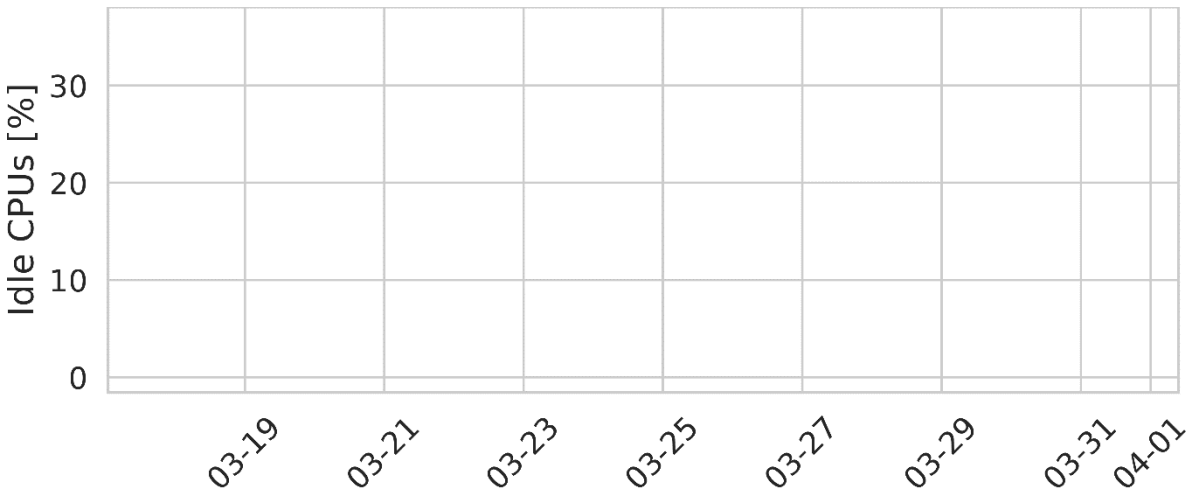
Tracking Wasted Resources in HPC



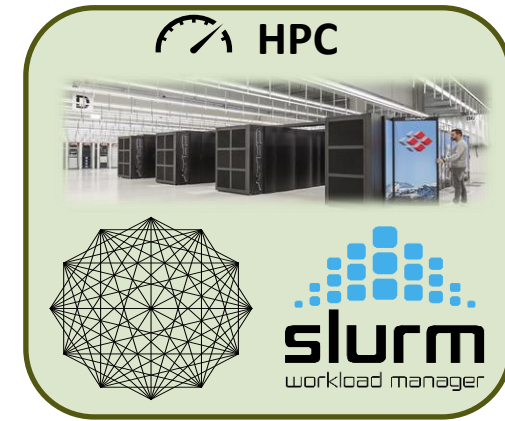
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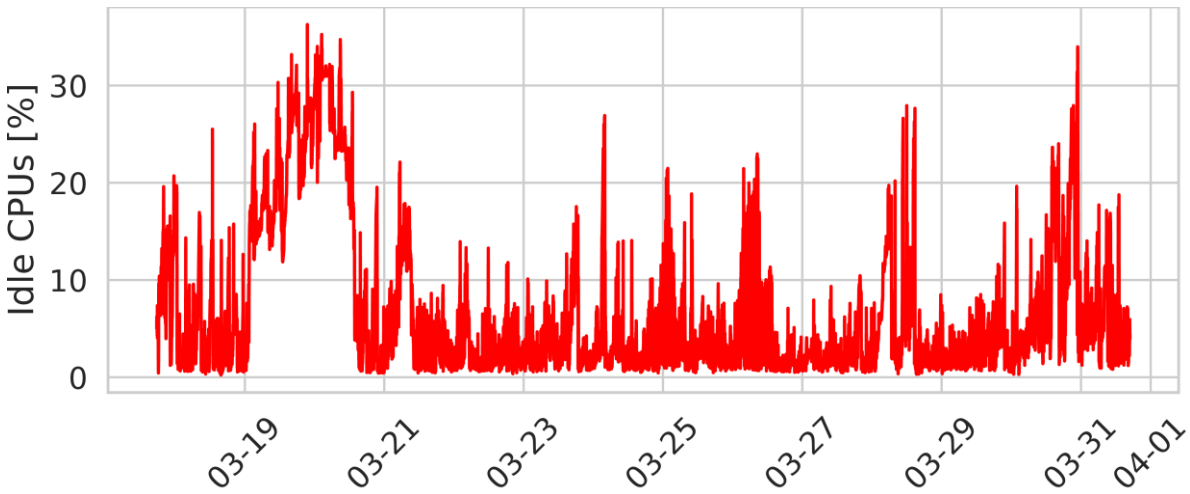
CPU



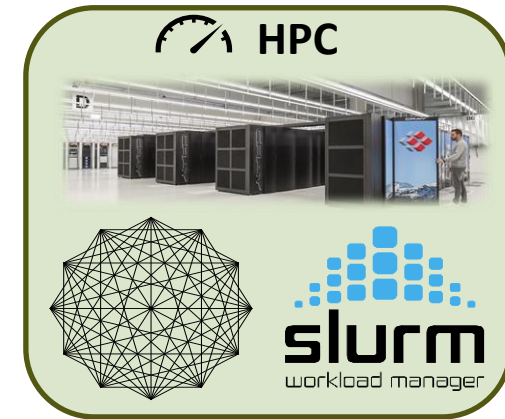
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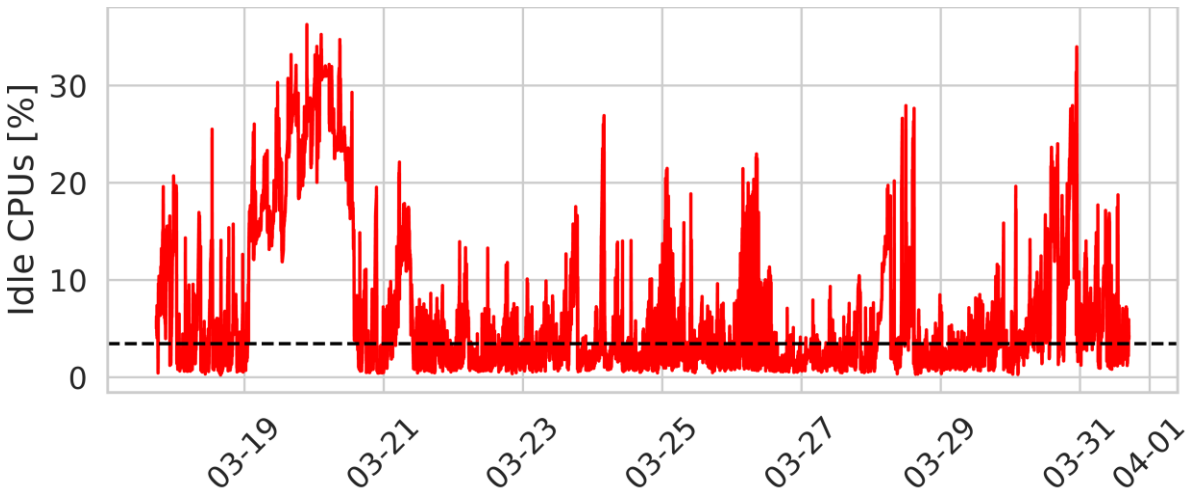
CPU



Tracking Wasted Resources in HPC

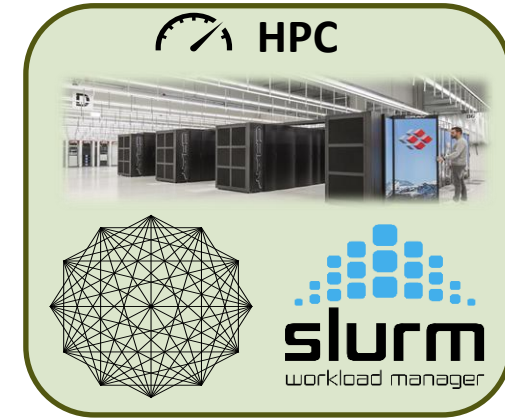


CPU

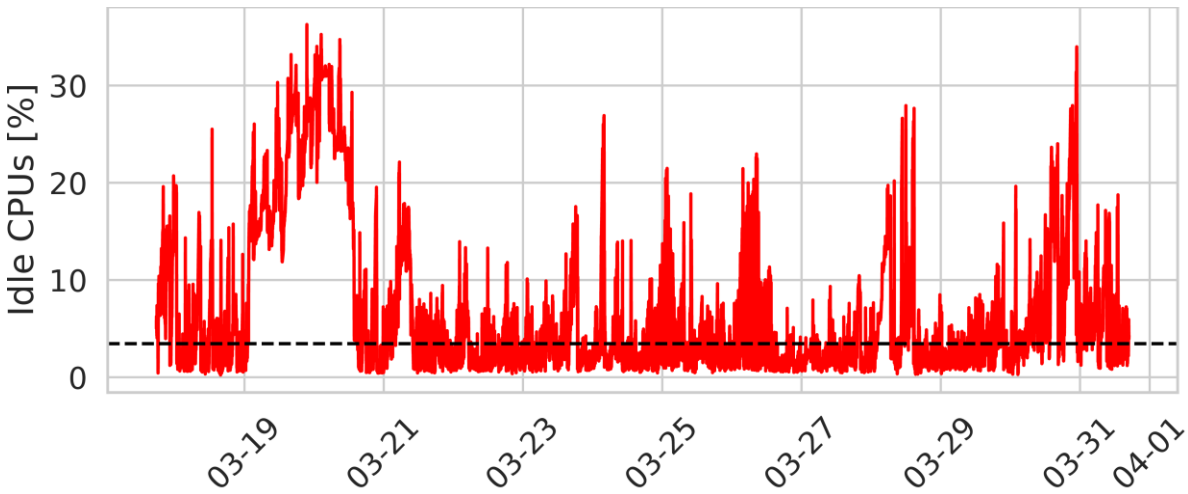


Mean idle CPUs: 6.6%

Tracking Wasted Resources in HPC

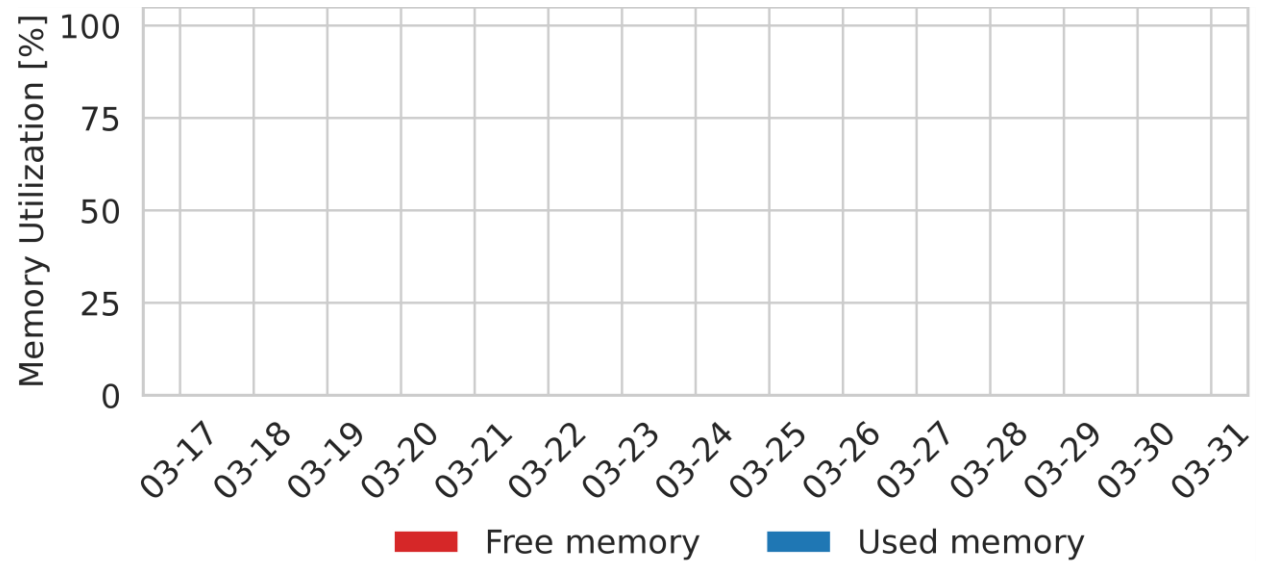


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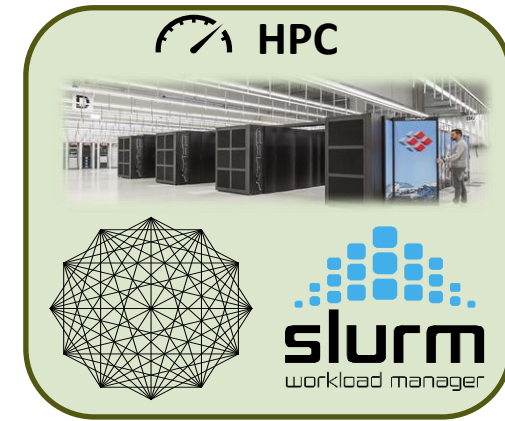


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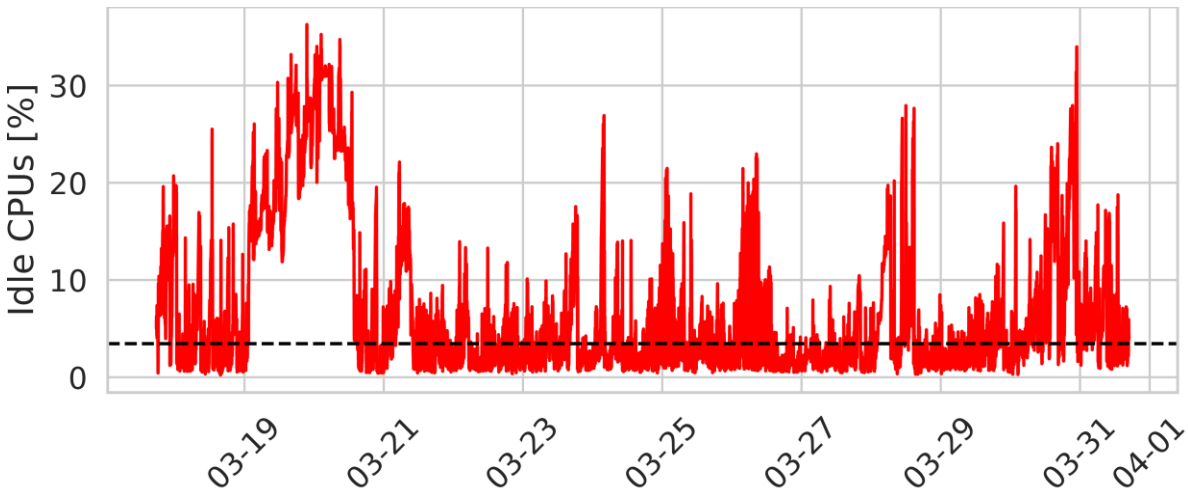
Memory



Tracking Wasted Resources in HPC

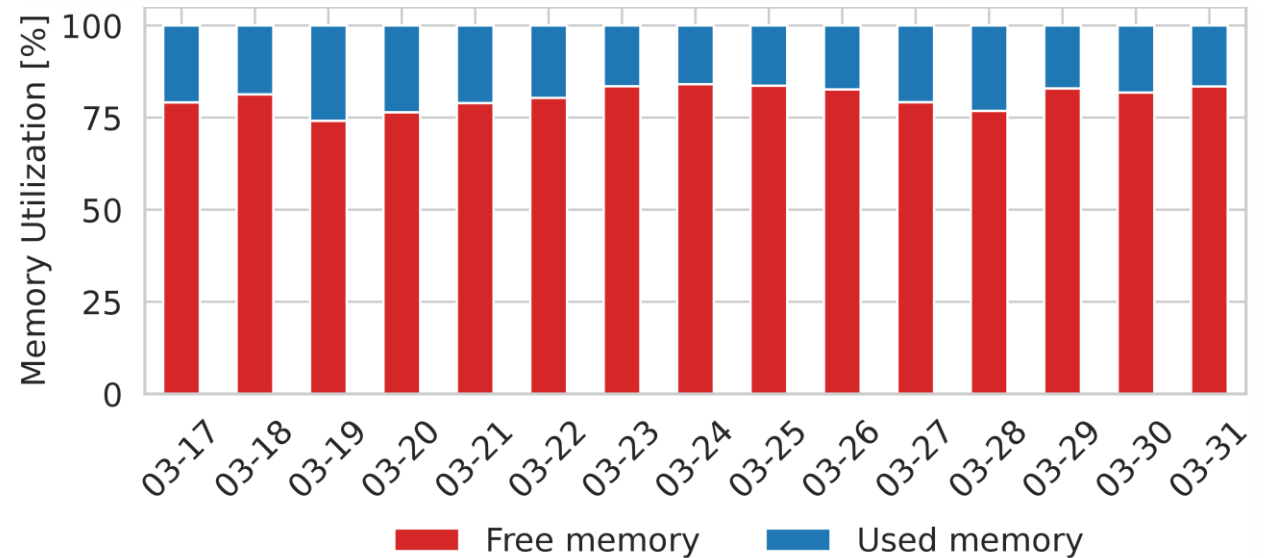


CPU



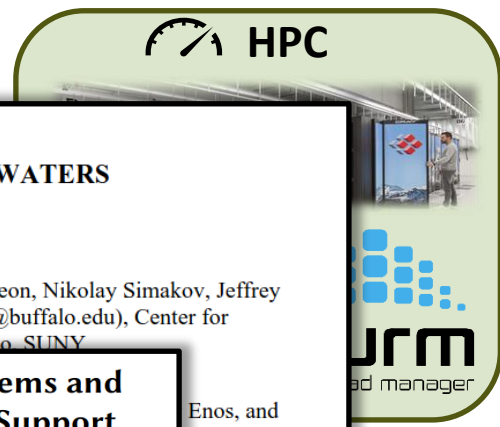
Mean idle CPUs: 6.6%

Memory



Mean free memory: 80.5%

Tracking Wasted Resources in HPC



Job Characteristics on Large-Scale Systems: Long-Term Analysis, Quantification, and Implications*

Tirthak Patel
Northeastern University

Zhengchun Liu, Raj Kettimuthu
Argonne National Laboratory

Paul Rich, William Allcock
Argonne National Laboratory

Devesh Tiwari
Northeastern University

SC, 2020

**FINAL REPORT
WORKLOAD ANALYSIS OF BLUE WATERS
(ACI 1650758)**

Matthew D. Jones, Joseph P. White, Martins Innus, Robert L. DeLeon, Nikolay Simakov, Jeffrey T. Palmer, Steven M. Gallo, and Thomas R. Furlani (furlani@buffalo.edu), Center for Computational Research, University at Buffalo, SUNY

Quantifying Memory Underutilization in HPC Systems and Using it to Improve Performance via Architecture Support

Gagandeep Panwar*
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Blacksburg, USA
gpanwar@vt.edu

Da Zhang*
Virginia Tech
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daz3@vt.edu

Yihan Pang*
Virginia Tech
Blacksburg, USA
pyihan1@vt.edu

A Case For Intra-rack Resource Disaggregation in HPC

GEORGE MICHELOGIANNAKIS, Lawrence Berkeley National Laboratory, USA

BENJAMIN KLENK, NVIDIA, USA

BRANDON COOK, Lawrence Berkeley National Laboratory, USA

Comprehensive Workload Analysis and Modeling of a Petascale Supercomputer

Haihang You¹ and Hao Zhang²

¹ National Institute for Computational Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

² Department of Electrical Engineering and Computer Science, University of Tennessee, Knoxville, TN 37996, USA

JSSPP, 2012

A Holistic View of Memory Utilization on HPC Systems: Current and Future Trends

Ivy B. Peng*
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ME

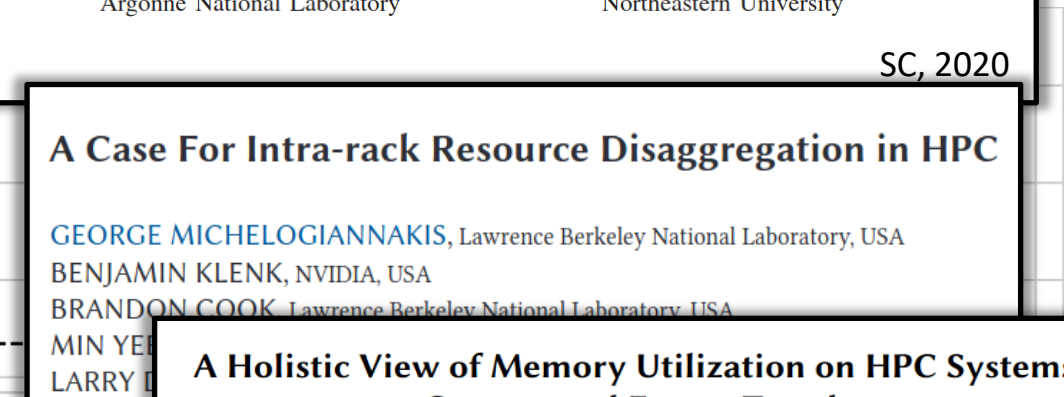
Learning from Five-year Resource-Utilization Data of Titan System

Feiyi Wang*, Sarp Oral†, Satyabrata Sen ‡ and Neena Imam§

Oak Ridge National Laboratory

CLUSTER, 2019

Idle CPUs [%]



Why C++ for Serverless?

Why C++ for Serverless?

Scientific Computing

rFaaS: Enabling High Performance Serverless with RDMA and Leases

Marcin Copik*, Konstantin Taranov[†], Alexandru Calotoiu*, Torsten Hoefler*

*Department of Computer Science, ETH Zürich, Zürich, Switzerland

[†]Microsoft

Why C++ for Serverless?

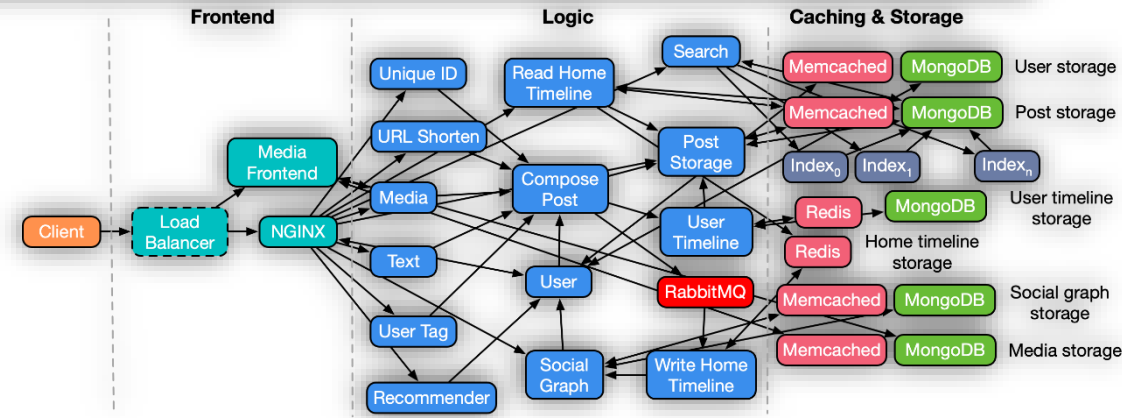
Scientific Computing

Microservices

Nightcore: Efficient and Scalable Serverless Computing for Latency-Sensitive, Interactive Microservices

Zhipeng Jia
The University of Texas at Austin
Austin, TX, USA
zjia@cs.utexas.edu

Emmett Witchel
The University of Texas at Austin
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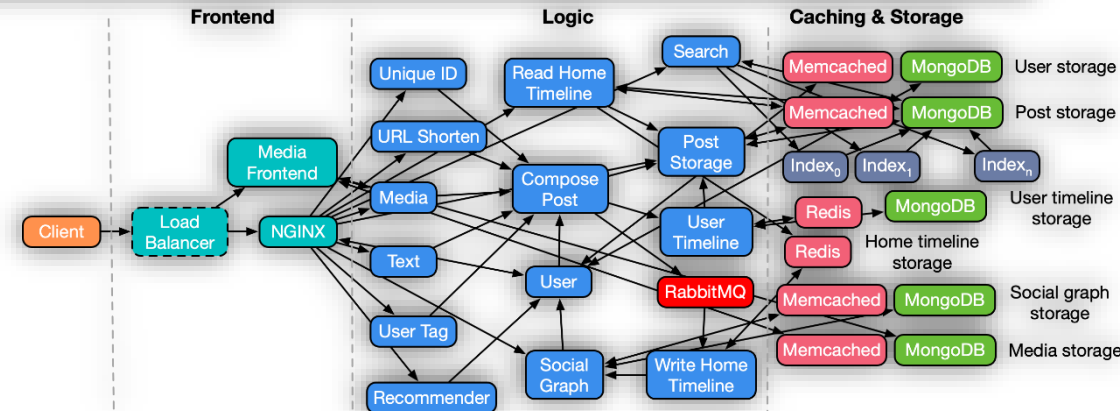
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†Microsoft

High-Performance Applications

R2E2: Low-Latency Path Tracing of Terabyte-Scale Scenes using Thousands of Cloud CPUs

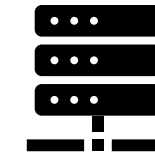
SADJAD FOULADI, Microsoft Research, USA and Stanford University, USA
BRENNAN SHACKLETT, FAIT POMS, ARJUN ARORA, ALEX OZDEMIR, DEEPTI RAGHAVAN, PAT HANRAHAN, KAYVON FATAHALIAN, and KEITH WINSTEIN, Stanford University, USA



FaaS Analysis: Invocation Overhead

 **User**

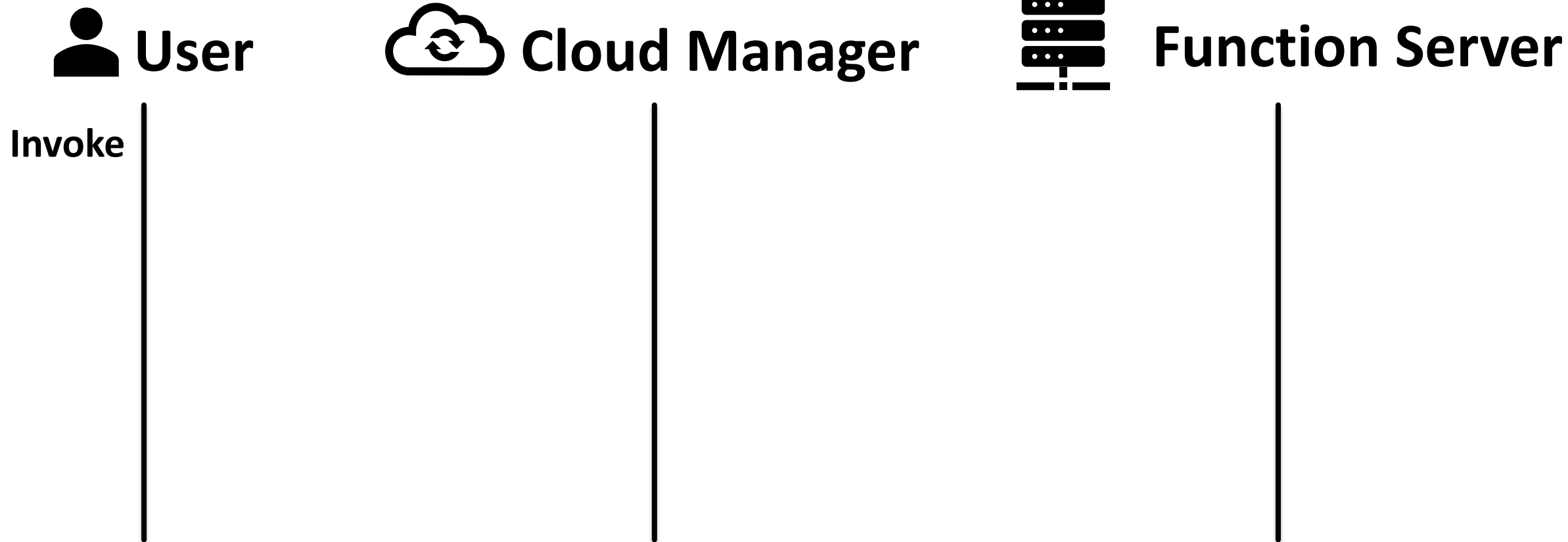
 **Cloud Manager**



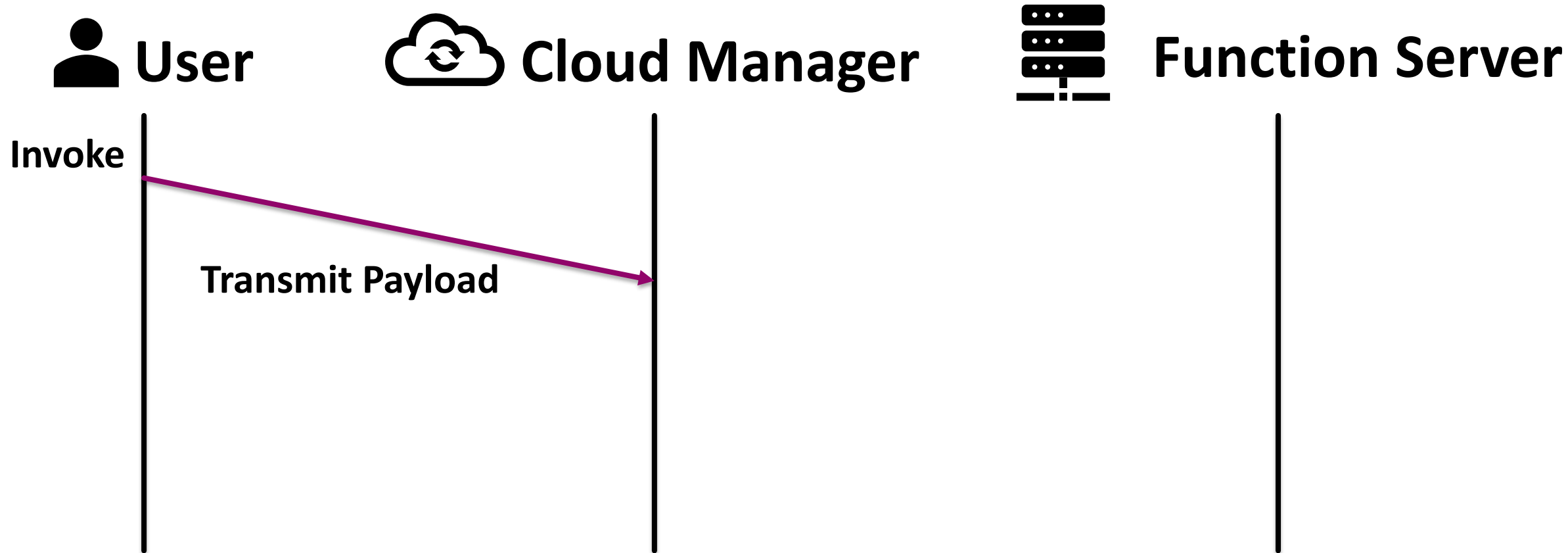
Function Server



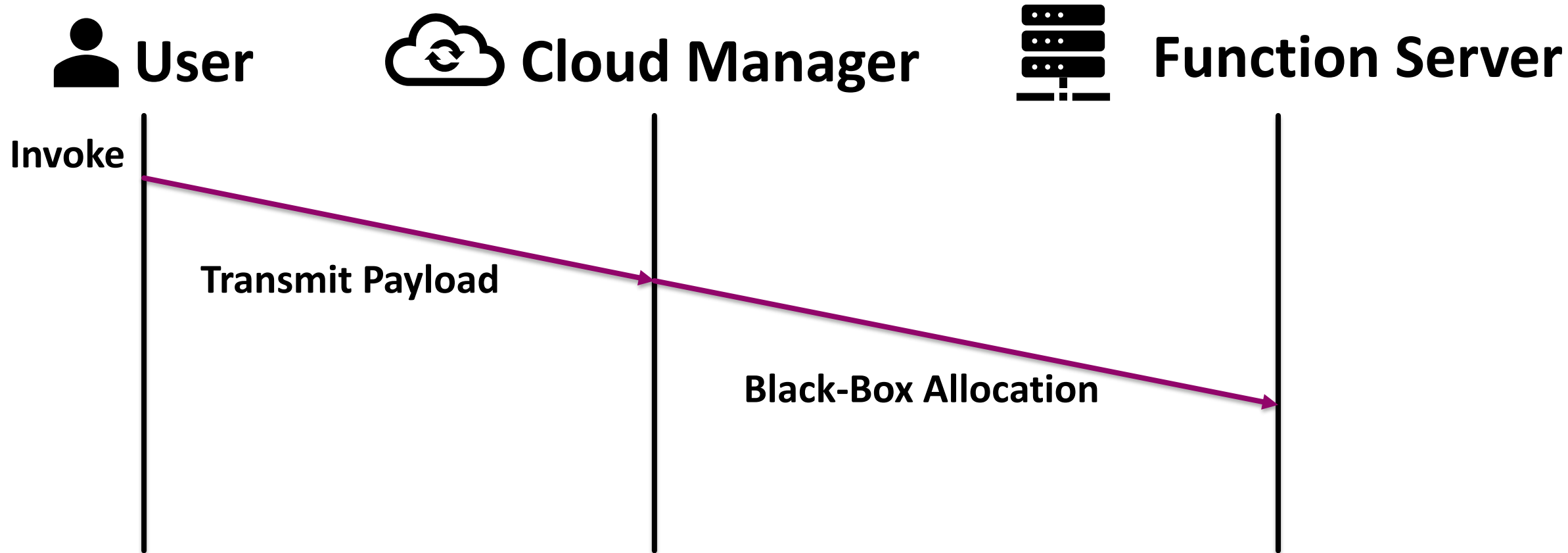
FaaS Analysis: Invocation Overhead



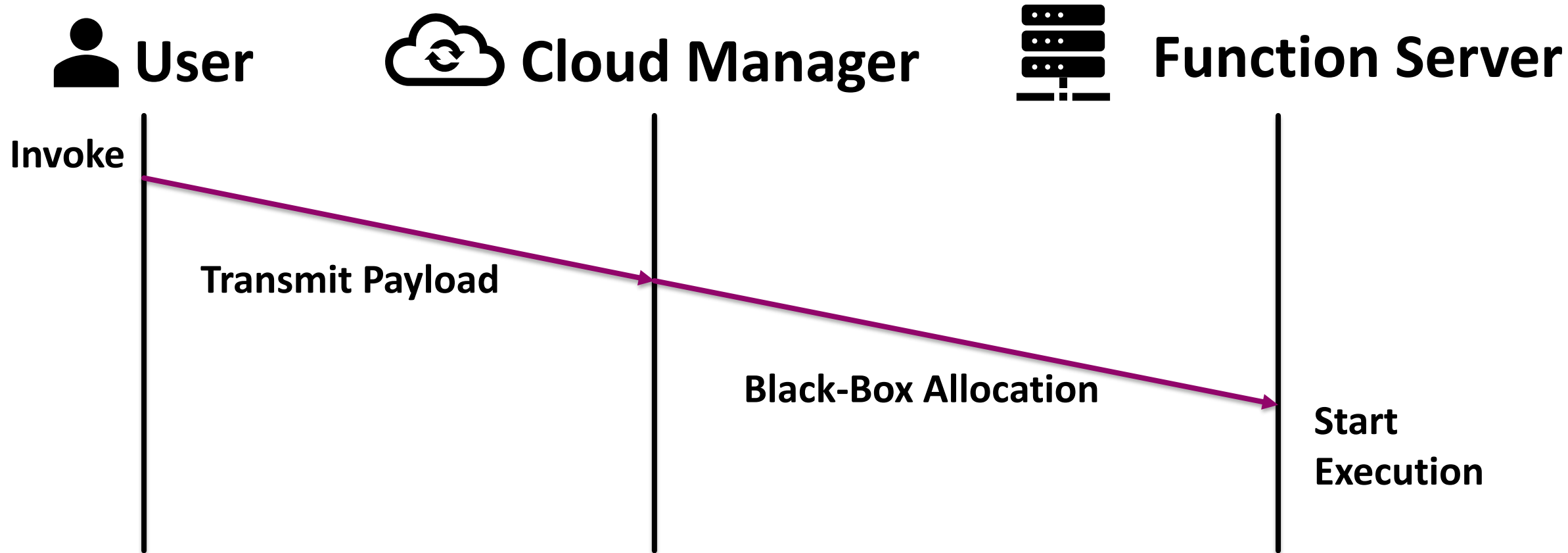
FaaS Analysis: Invocation Overhead



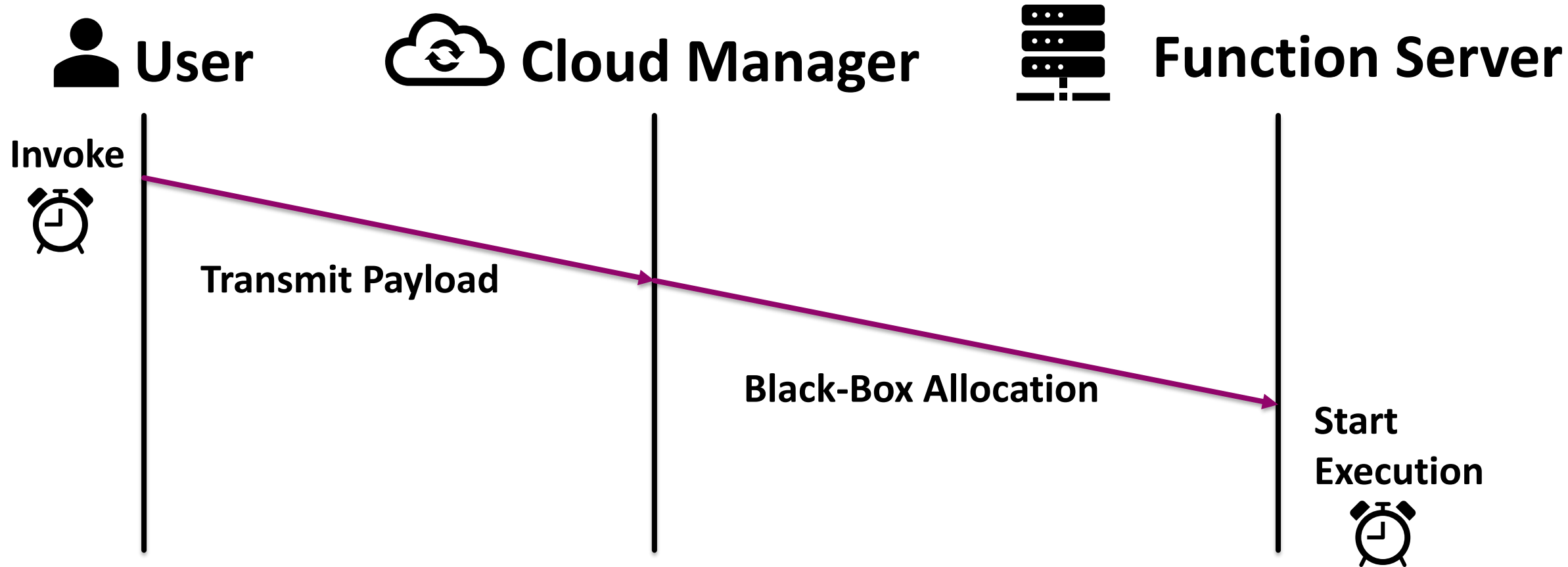
FaaS Analysis: Invocation Overhead



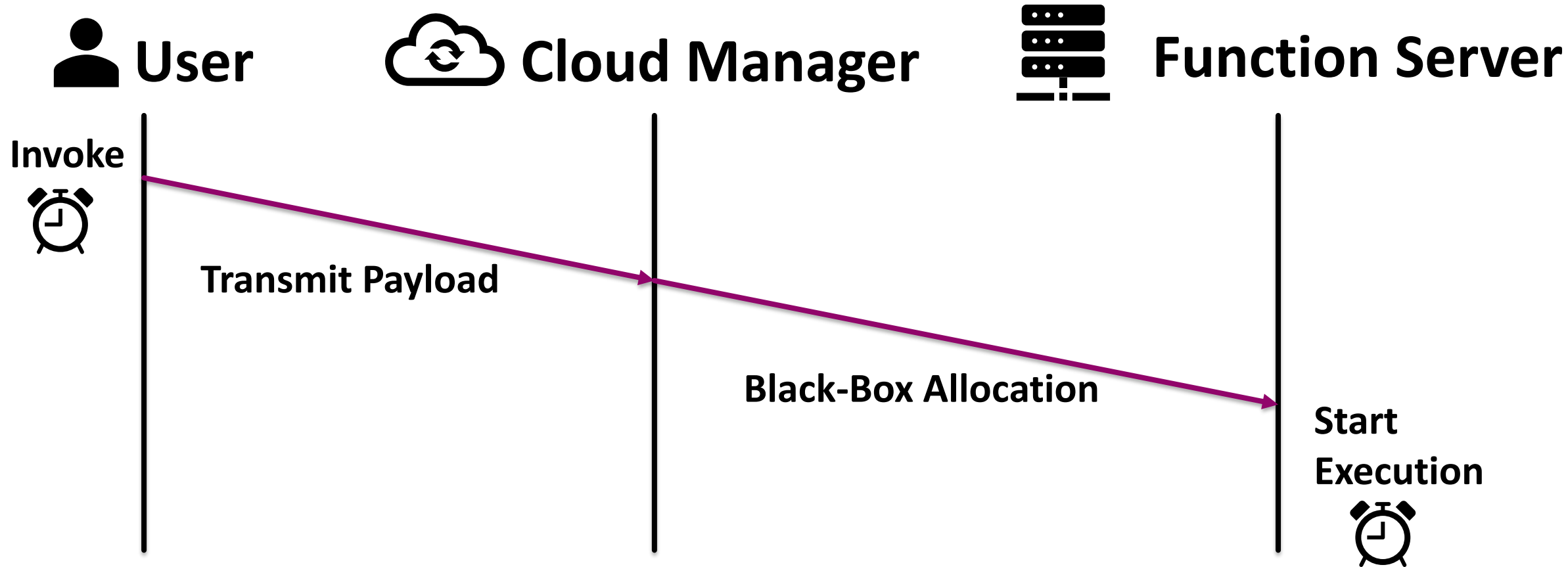
FaaS Analysis: Invocation Overhead



FaaS Analysis: Invocation Overhead



FaaS Analysis: Invocation Overhead



Solution: apply clock-drift estimation protocols!

“SeBS: a Serverless Benchmark Suite for Function-as-a-Service Computing”, Middleware 2021

FaaS Analysis: Invocation Overhead



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FaaS Analysis: Invocation Overhead

Configuration:

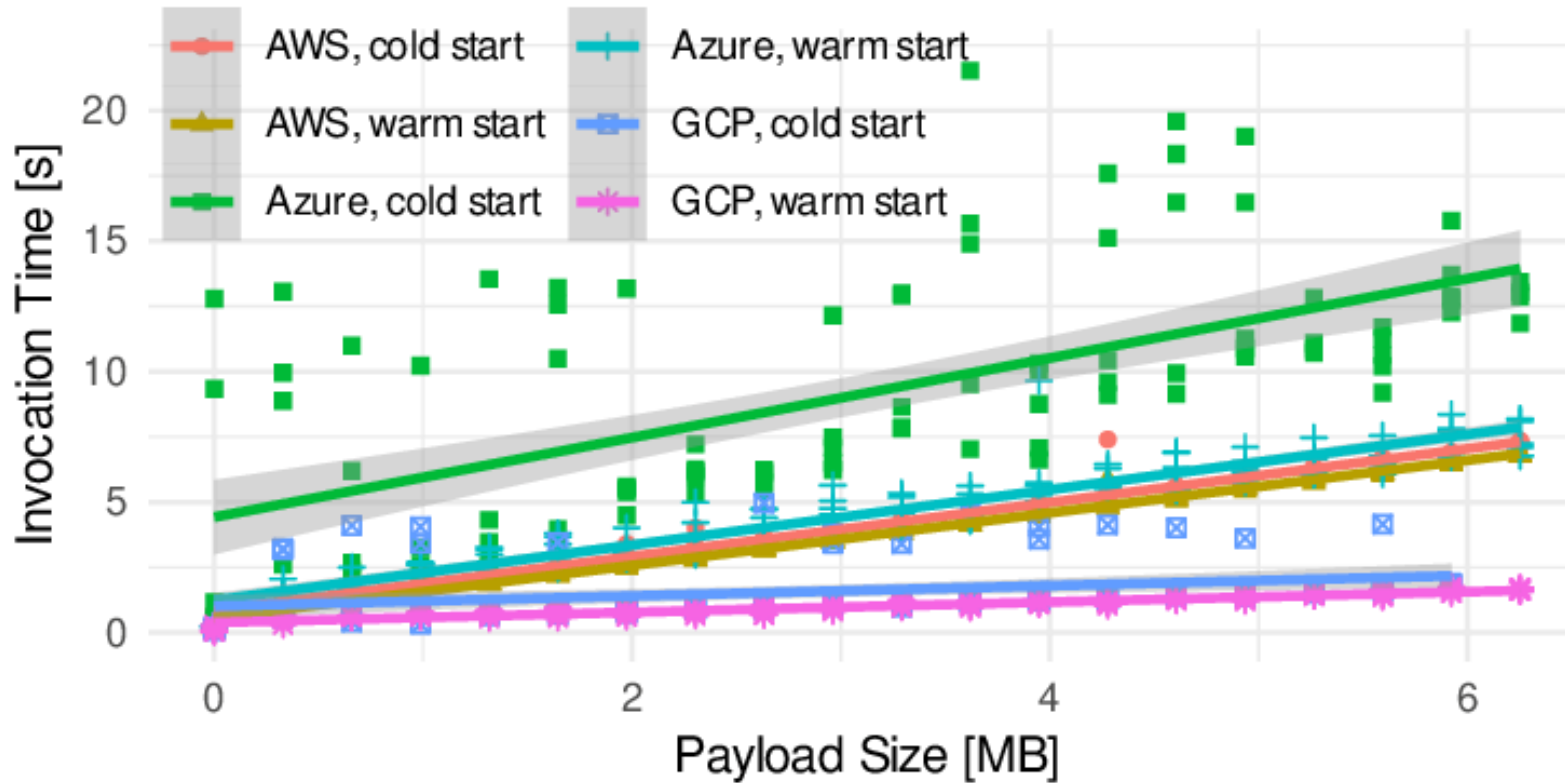
- Compare timestamps on client and function side.
- Clock drift estimation protocol.
- Payload: 1 kB – 5.9 MB



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SeBS-Flow: Let the Work Flow in the Cloud



“SeBS-Flow: Benchmarking Serverless Cloud Function Workflows”, Schmid et al., EuroSys 2025



SeBS-Flow: Let the Work Flow in the Cloud

Analysis of 72 research papers: how are serverless workflows evaluated?

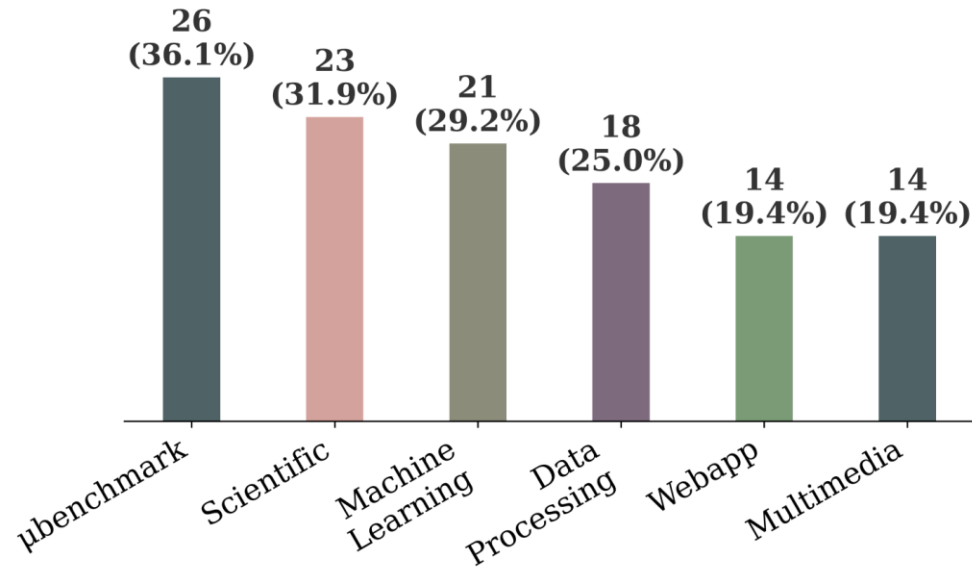


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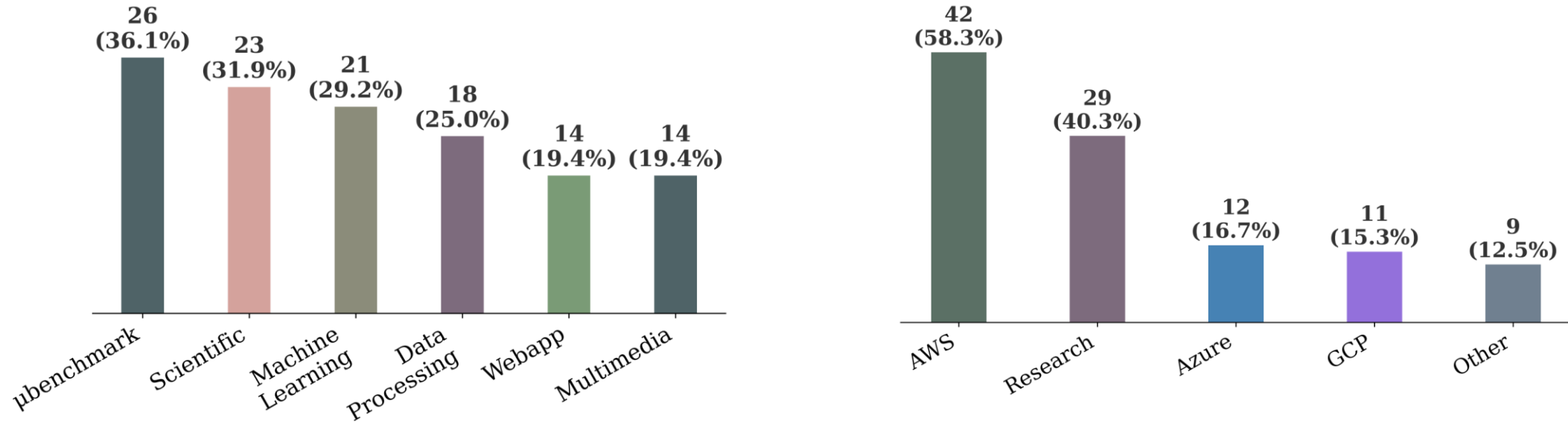


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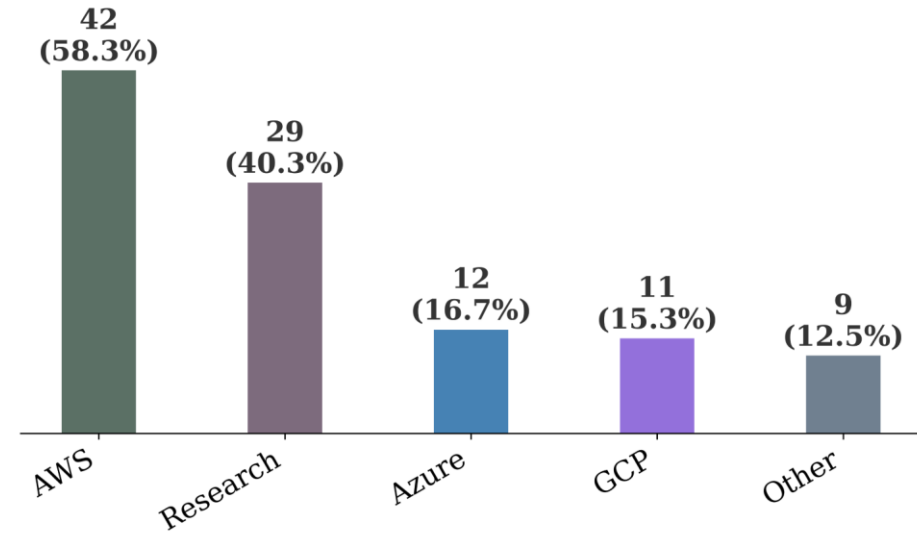
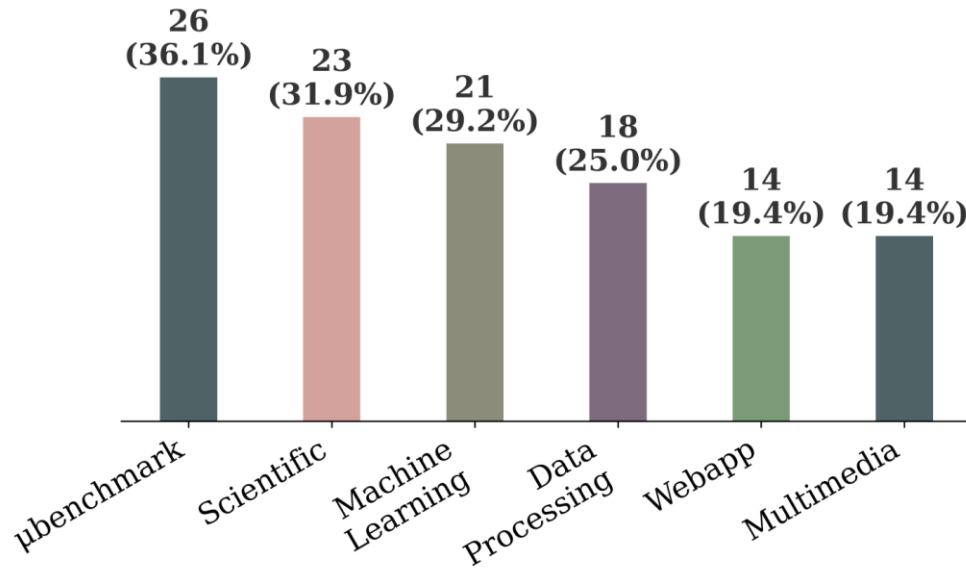


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AWS Step Functions



Azure Durable Functions

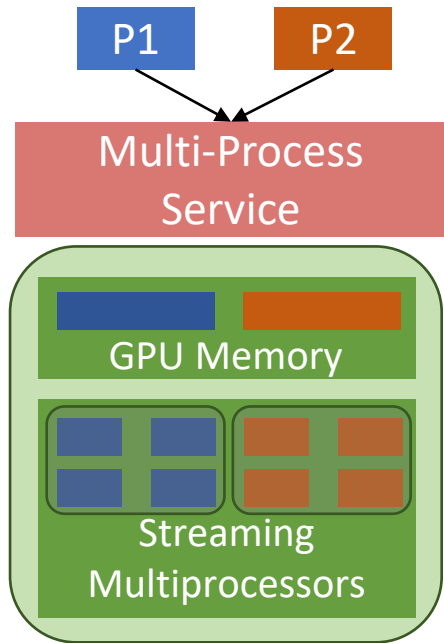


Google Cloud Workflows

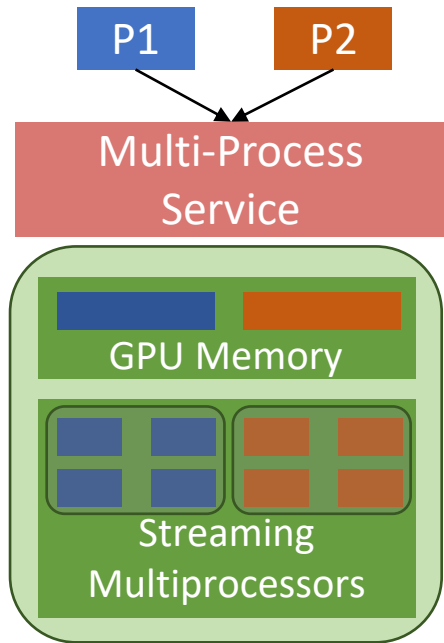


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Serverless GPUs: Multi-Process Service (MPS) to the Rescue?

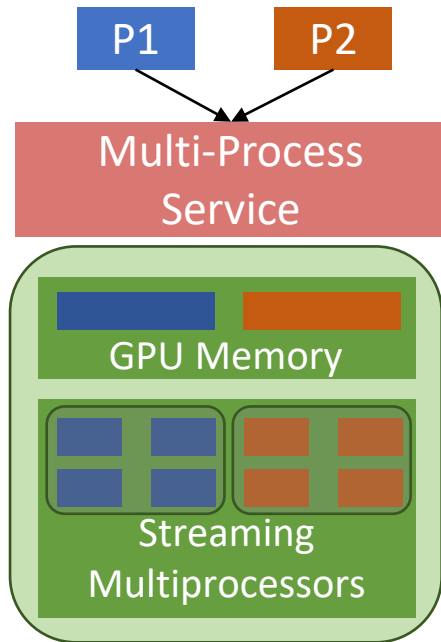


Serverless GPUs: Multi-Process Service (MPS) to the Rescue?



“MPS is only recommended for running **cooperative processes** effectively acting as a **single application**, such as multiple ranks of the same MPI job, such that the severity of the following memory protection and error containment limitations is acceptable.”

Serverless GPUs: Multi-Process Service (MPS) to the Rescue?

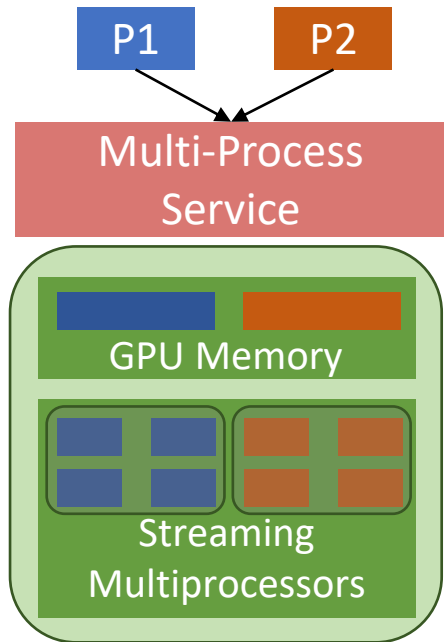


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Serverless is multi-tenant and executes arbitrary user code.

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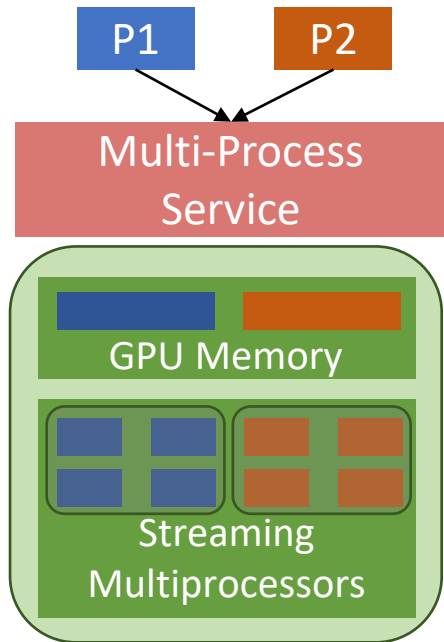
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Limited security!

Function can conduct side-channel attack.

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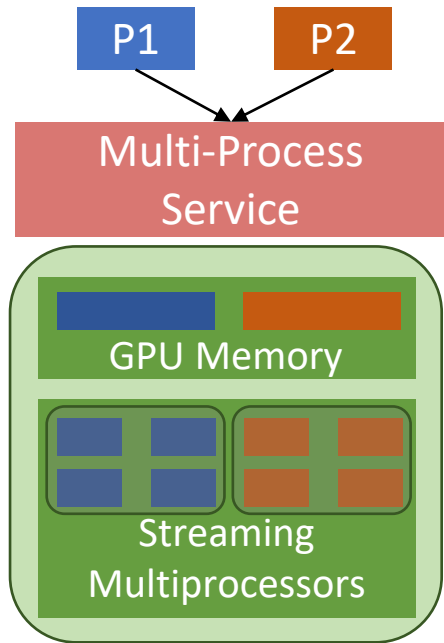
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Serverless is multi-tenant and executes arbitrary user code.



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No performance isolation!

Function can hog the memory bandwidth.



No error containment!

Function can maliciously kill GPU contexts.

Serverless GPUs: Building from Blocks with Multi-Instance GPU (MIGs)

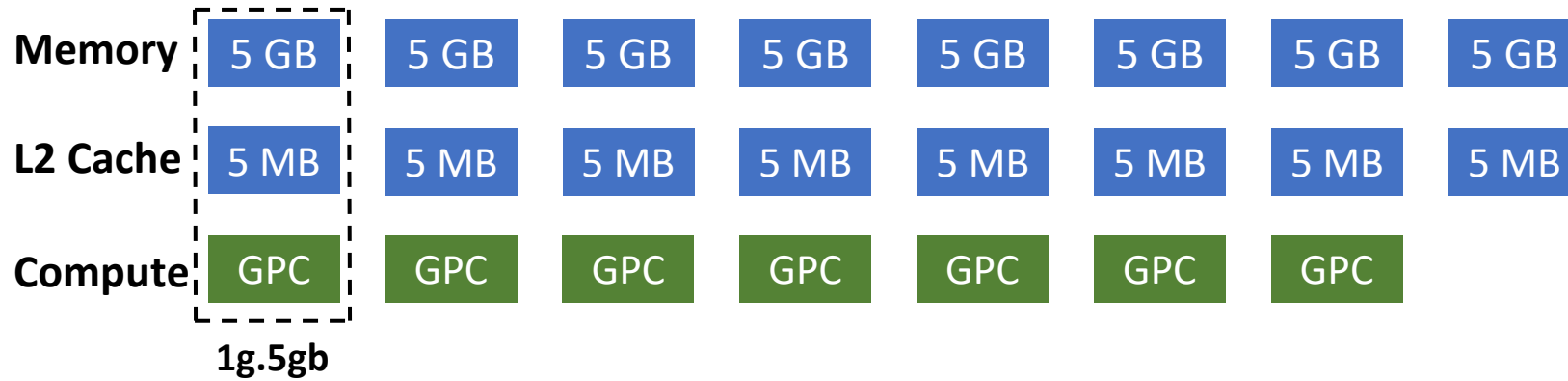
Serverless GPUs: Building from Blocks with Multi-Instance GPU (MIGs)

Memory	5 GB	5 GB	5 GB	5 GB	5 GB	5 GB	5 GB	5 GB
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Memory	5 GB	5 GB	5 GB	5 GB	5 GB	5 GB	5 GB	5 GB
L2 Cache	5 MB	5 MB	5 MB	5 MB	5 MB	5 MB	5 MB	5 MB
Compute	GPC	GPC	GPC	GPC	GPC	GPC	GPC	GPC

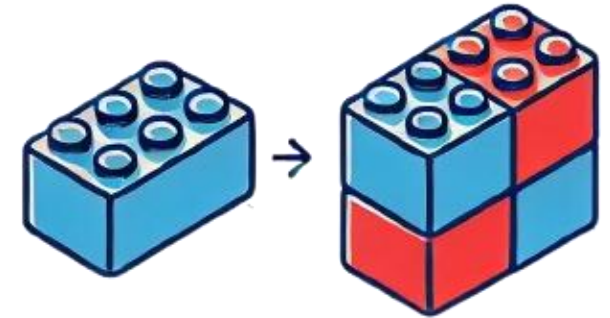
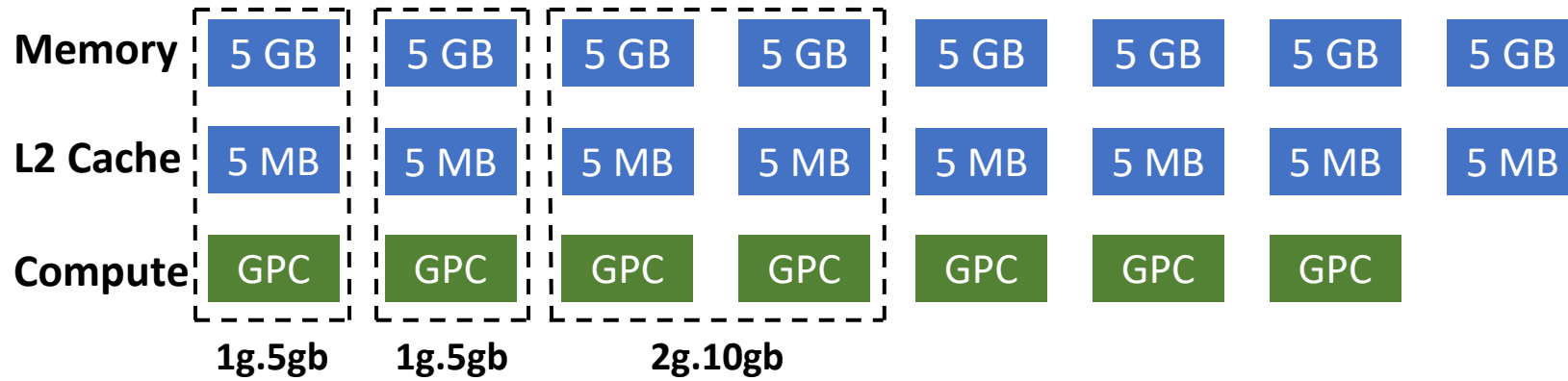
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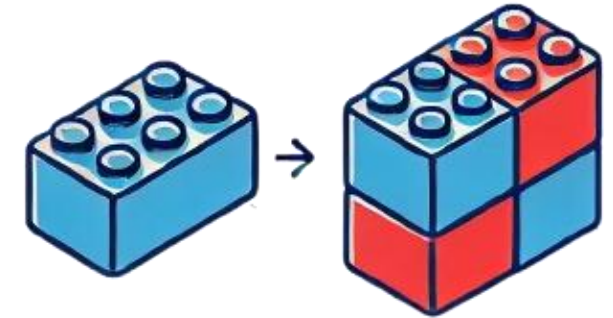
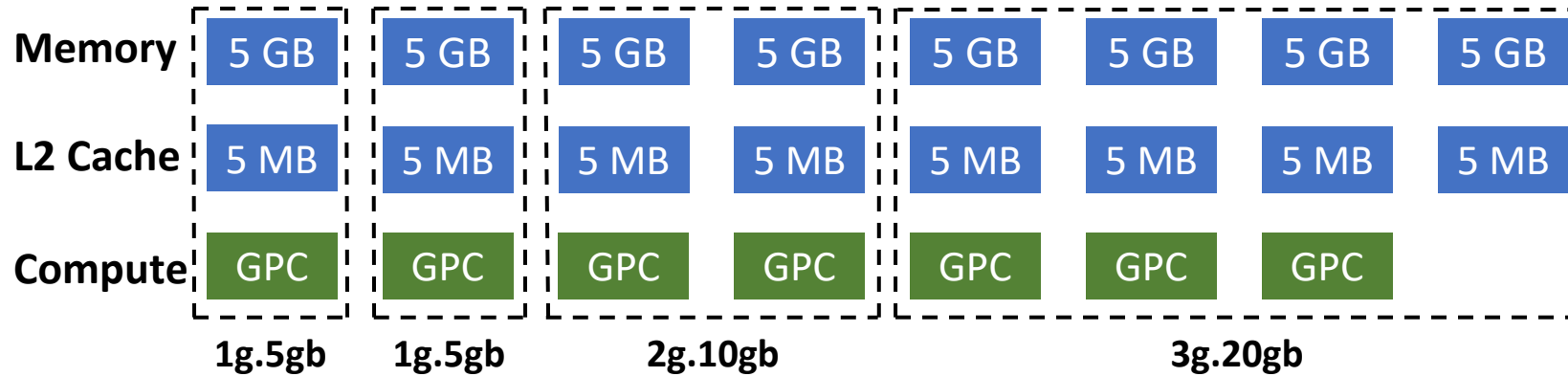
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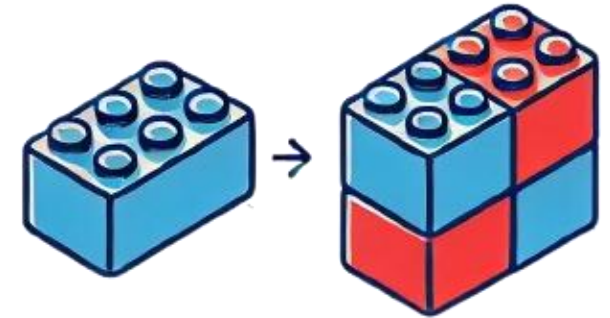
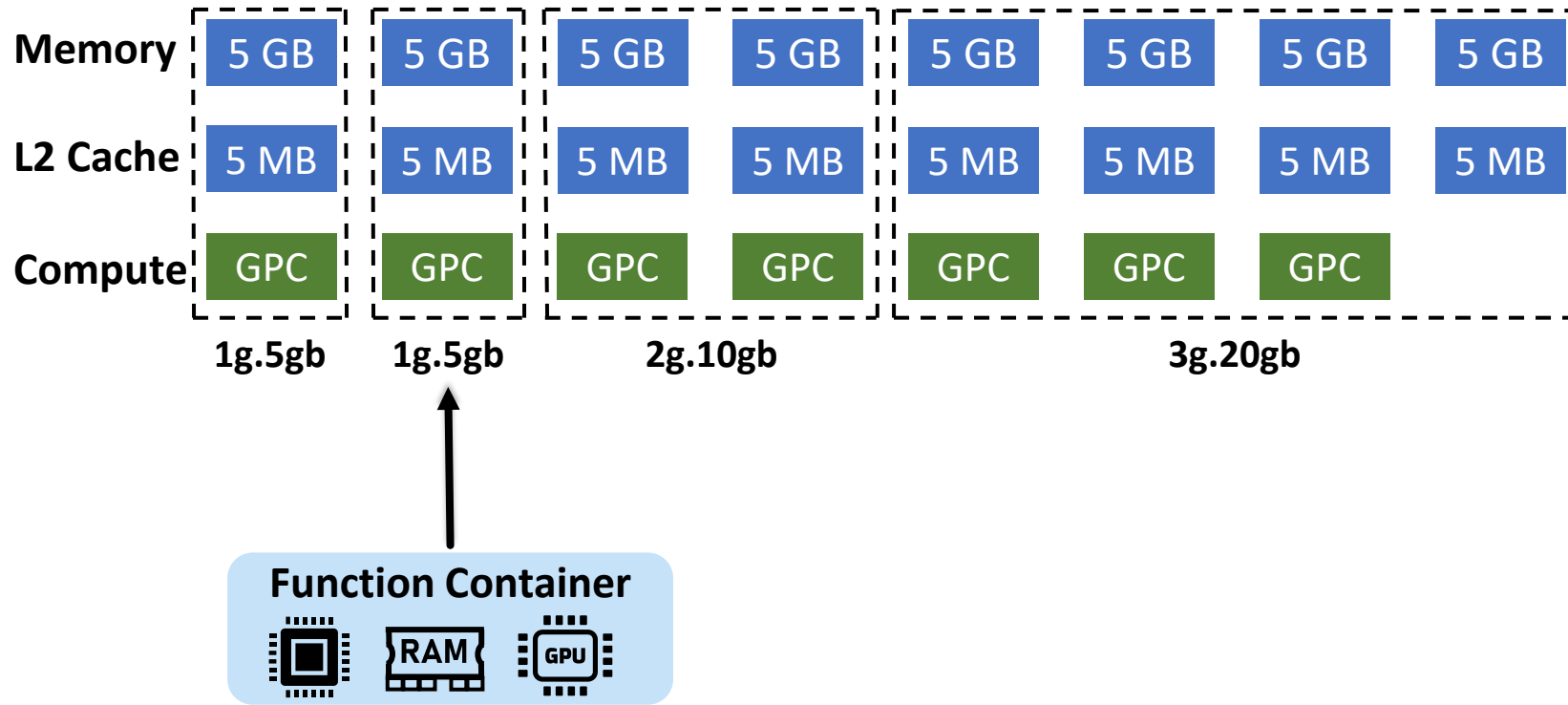
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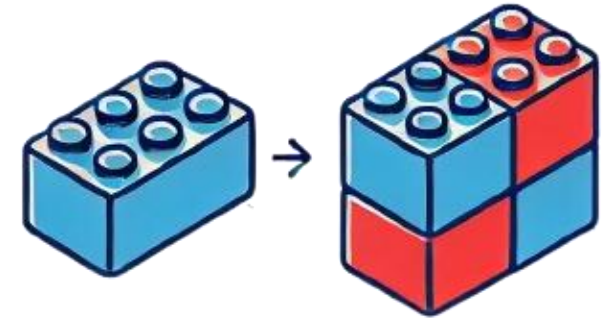
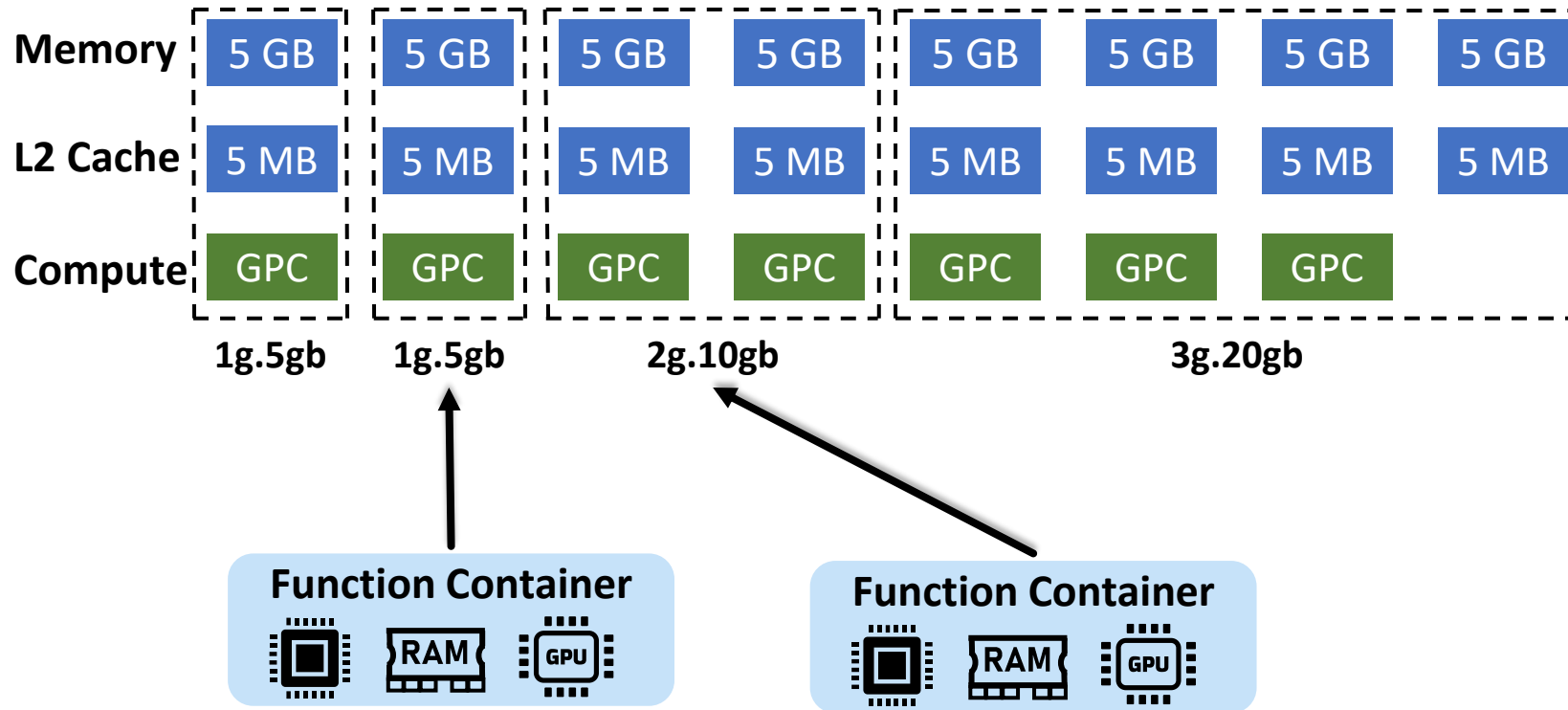
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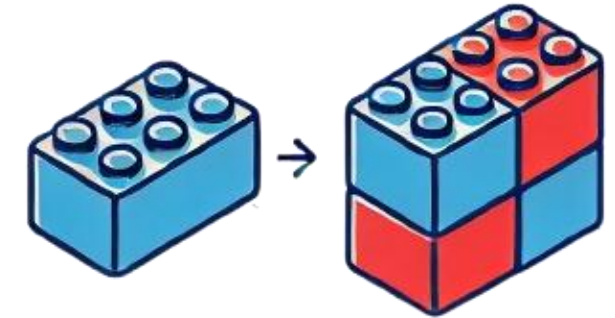
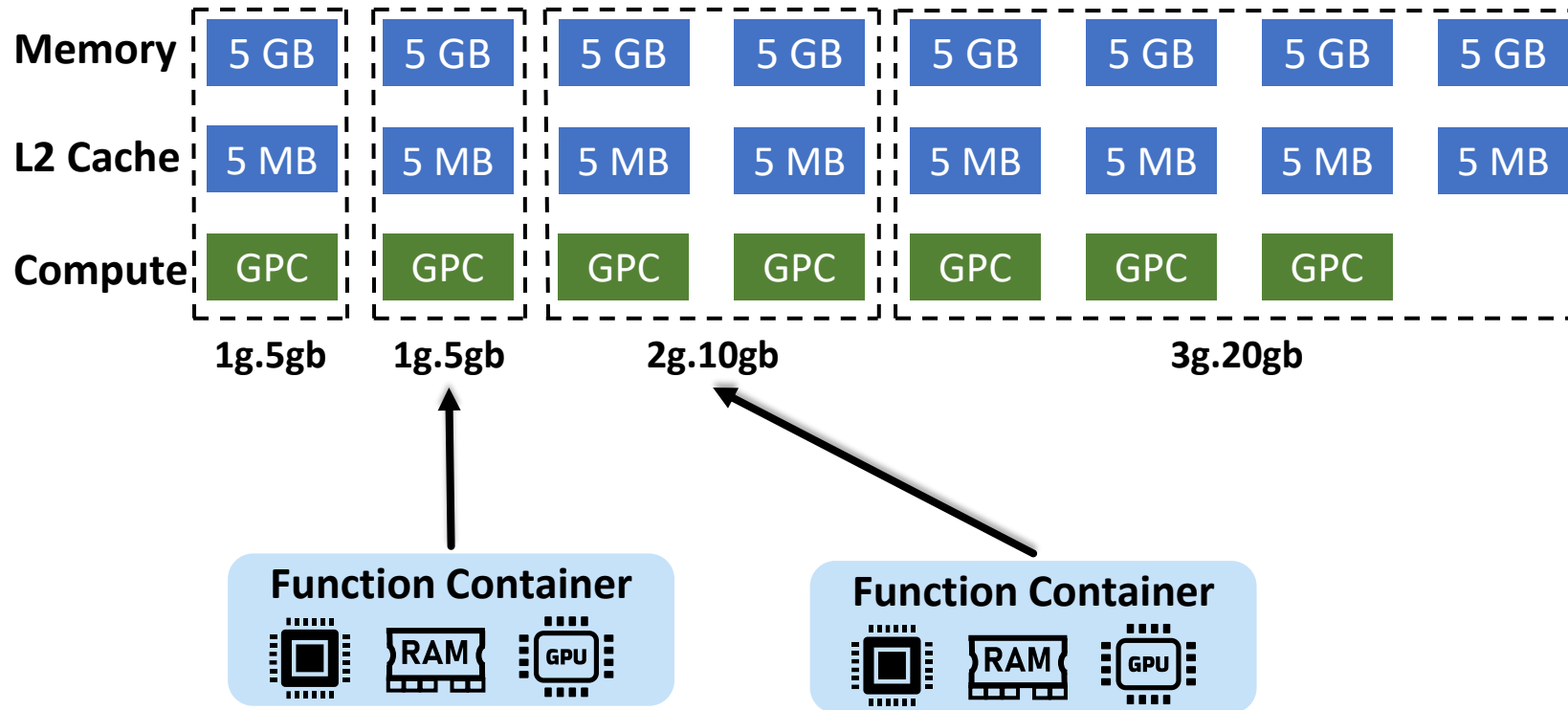
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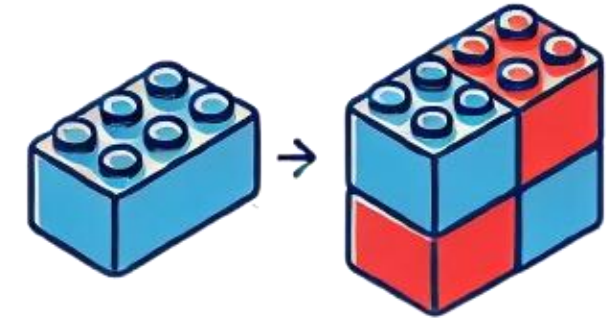
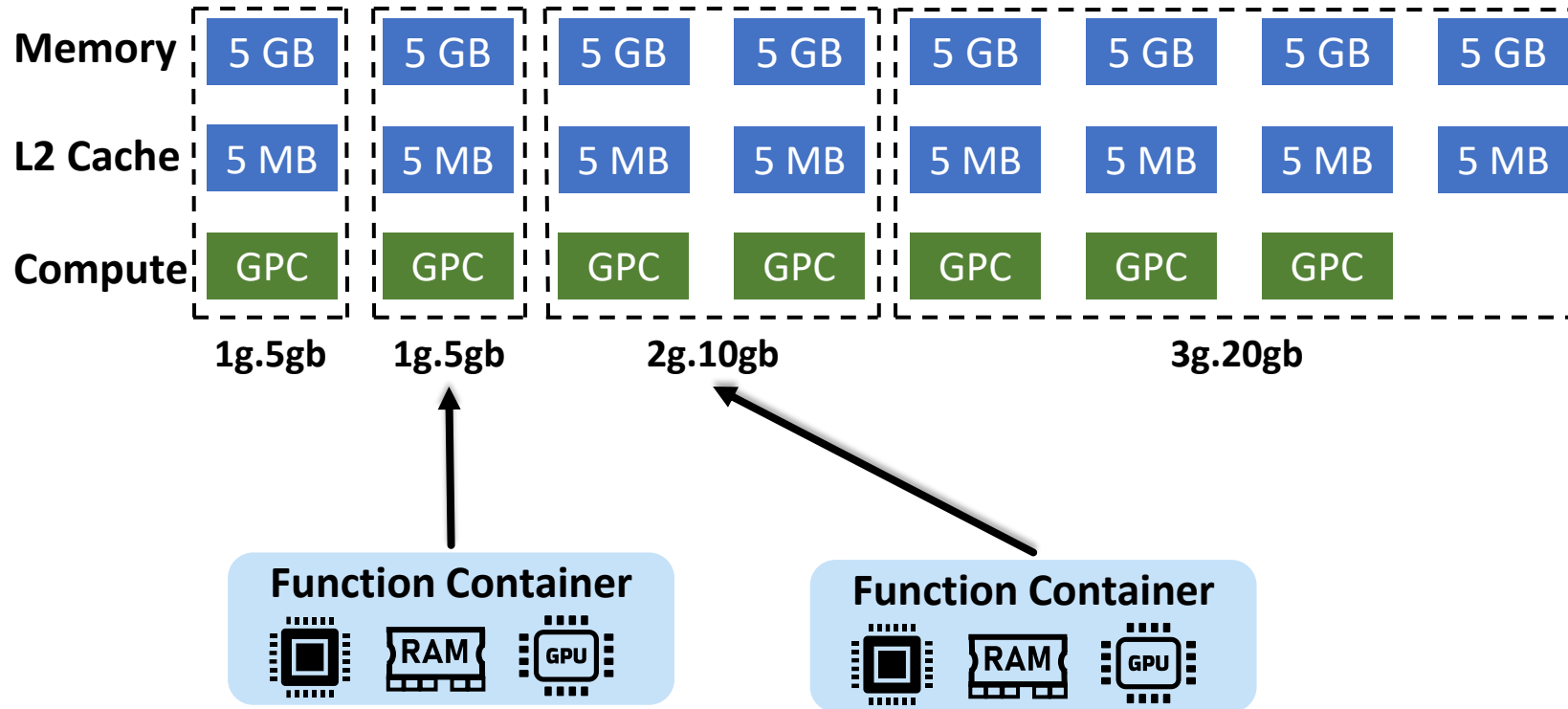


Serverless GPUs: Building from Blocks with Multi-Instance GPU (MIGs)



Not elastic!
Partitioning is quite static.

Serverless GPUs: Building from Blocks with Multi-Instance GPU (MIGs)



Not elastic!
Partitioning is quite static.



Static underutilization!
Difficult to migrate between partitions.

Evaluation – GROMACS Performance Portability

Why not just build one SYCL container for CUDA and Intel GPUs?

Installation guide for exotic configurations

Special instructions for building GROMACS on less-common systems

These instructions pertain to building GROMACS 2025.2. This document is complementary to the [up-to-date installation instructions](#) instructions.

The configurations listed here are expected to work, but are not recommended for typical users.

SYCL GPU acceleration for AMD and NVIDIA GPUs using Intel oneAPI DPC++

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15-20% slowdown
on test case A

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**Needs compile-time
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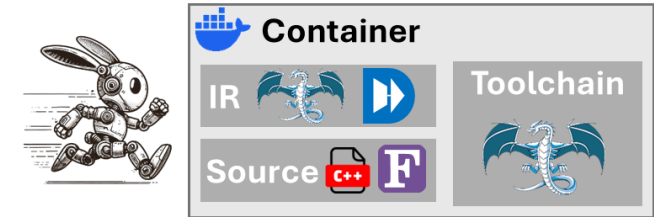


Failure on test case B

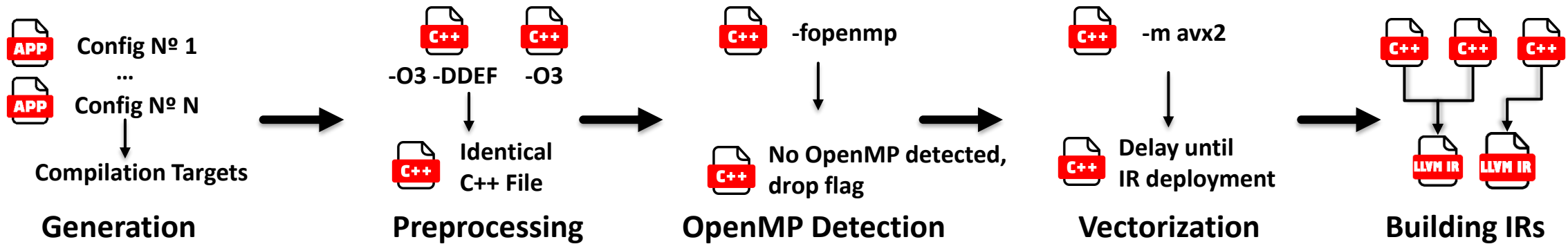


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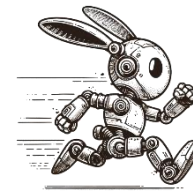
XaaS IR Containers: Build Containers







XaaS IR Container

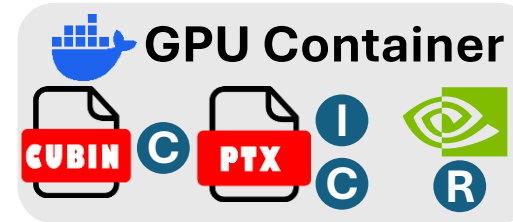


XaaS IR Container



	IR Files
	Source Code
	Dependencies
	Toolchain

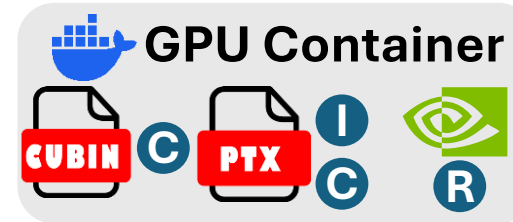
XaaS IR Containers: GPU Acceleration



XaaS IR Containers: GPU Acceleration

CUDA Compatibility Model

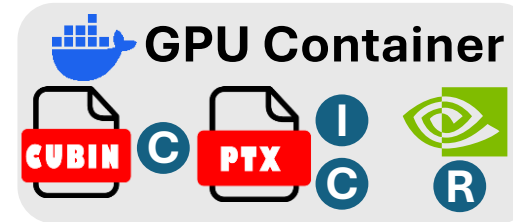
- D** Driver Version



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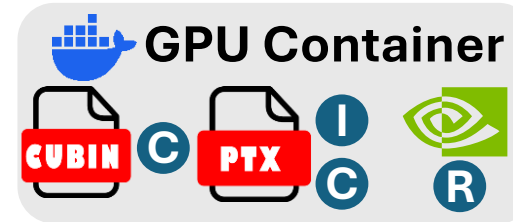
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XaaS IR Containers: GPU Acceleration

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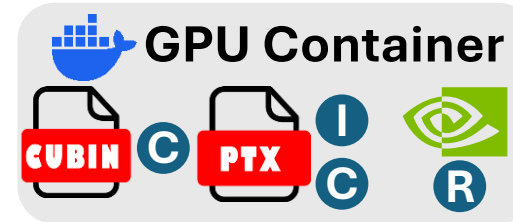
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XaaS IR Containers: GPU Acceleration

CUDA Compatibility Model

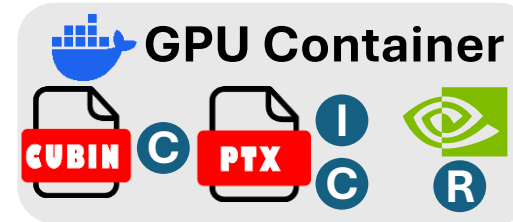
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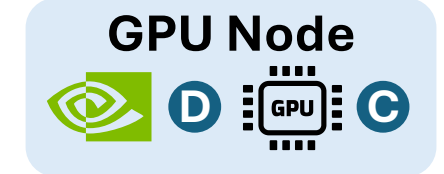
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Deploy

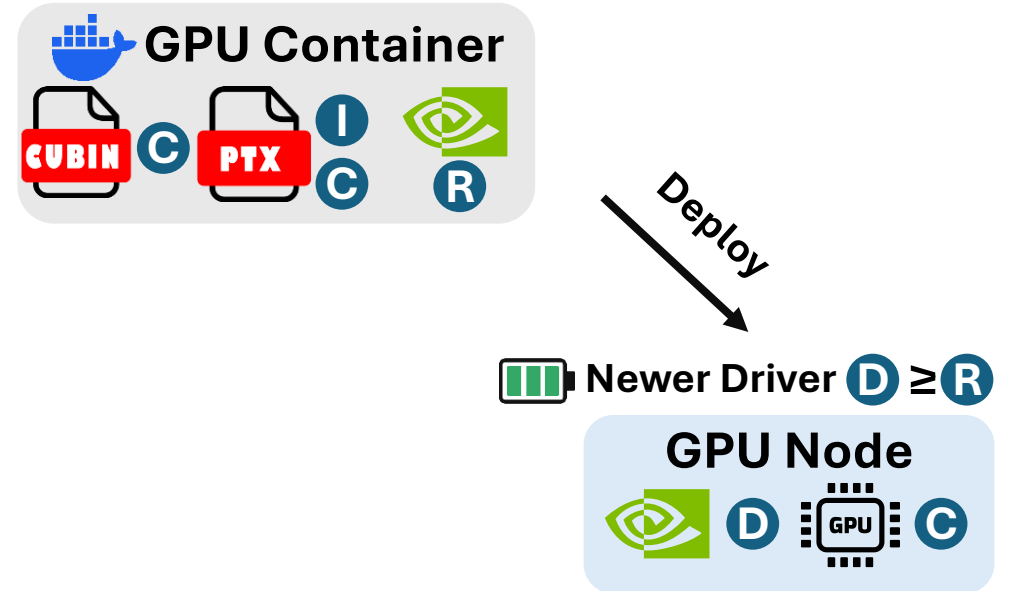
Newer Driver $D \geq R$



XaaS IR Containers: GPU Acceleration

CUDA Compatibility Model

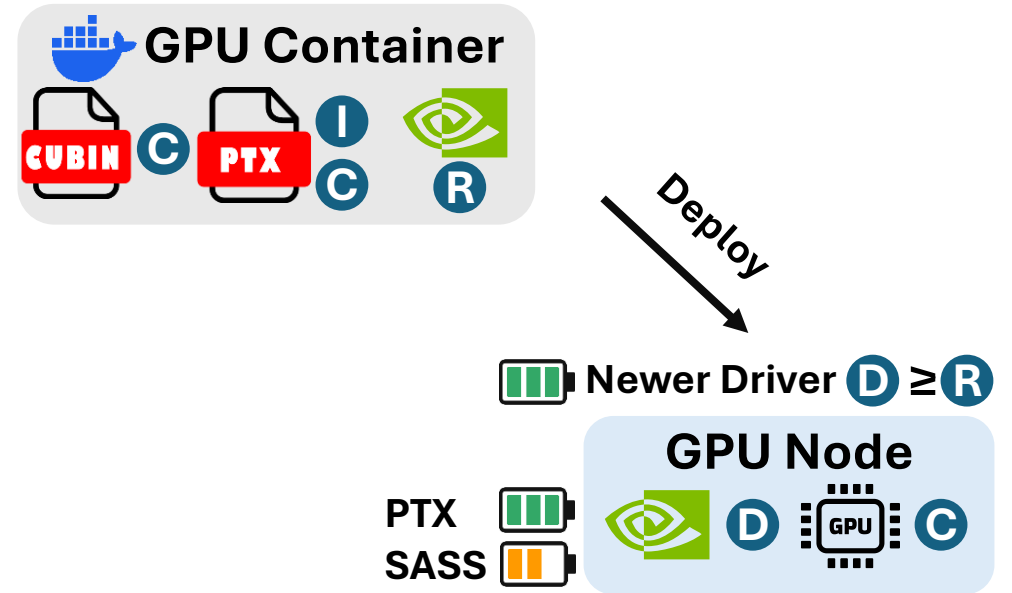
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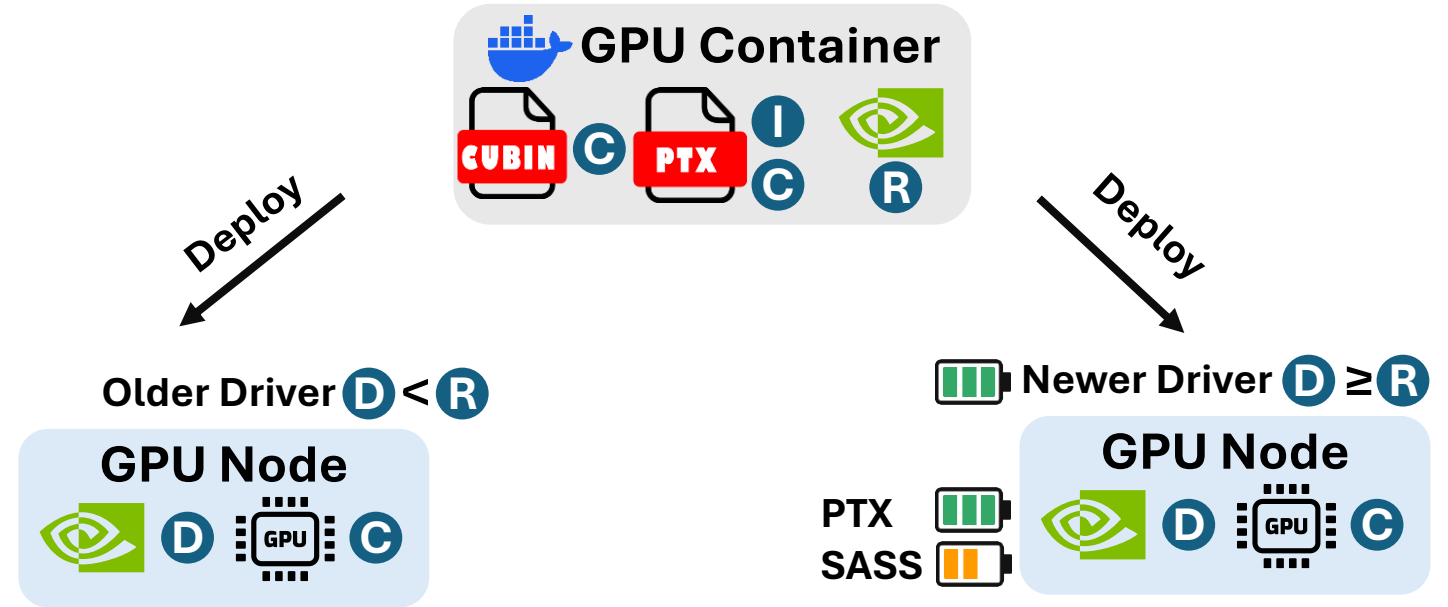
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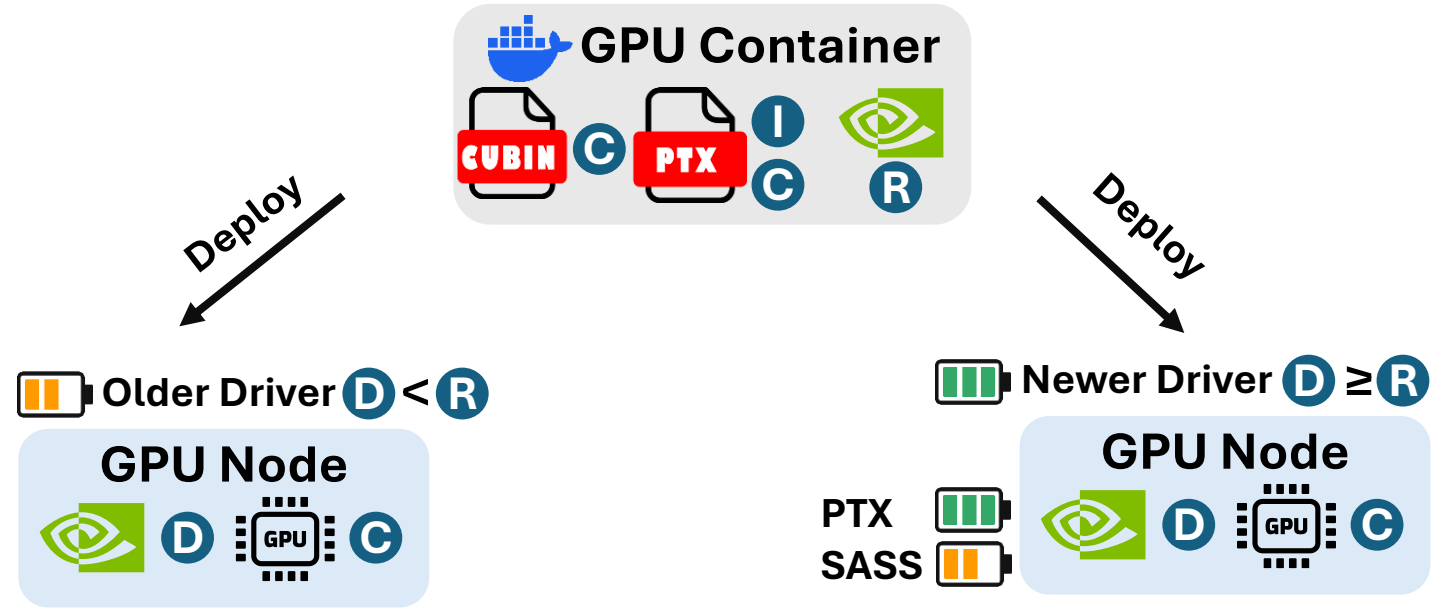
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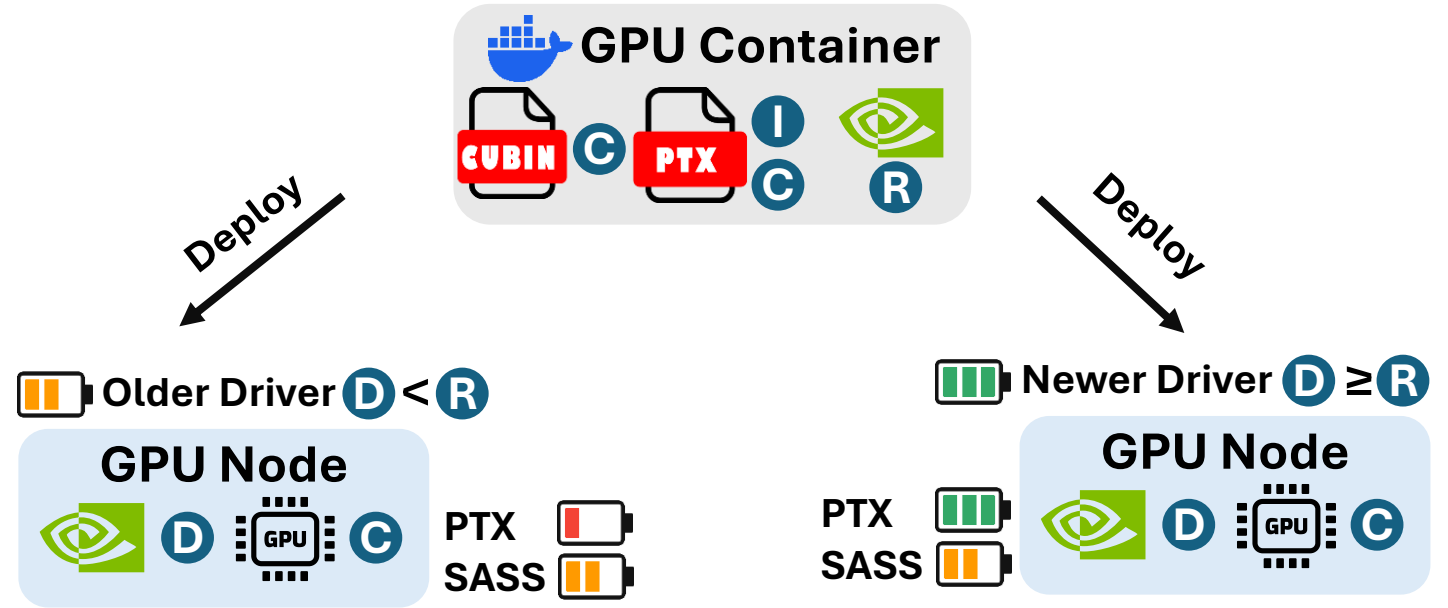
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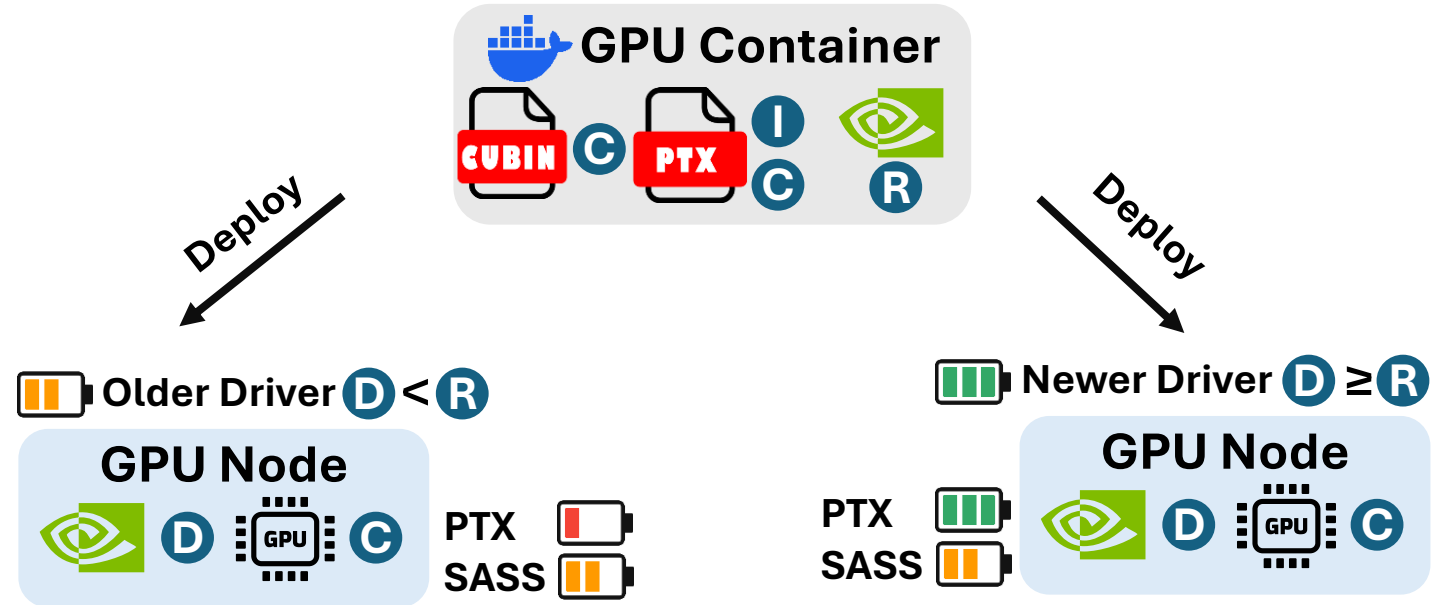
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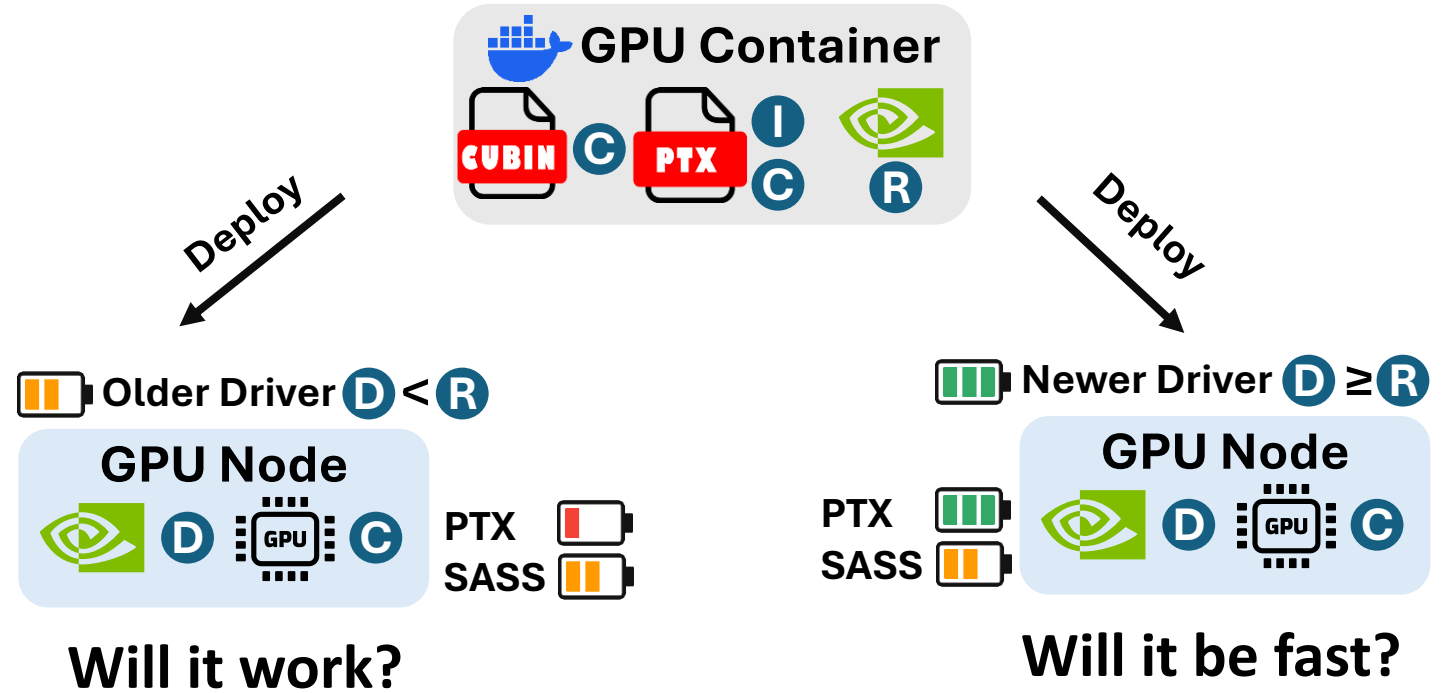


Will it work?

XaaS IR Containers: GPU Acceleration

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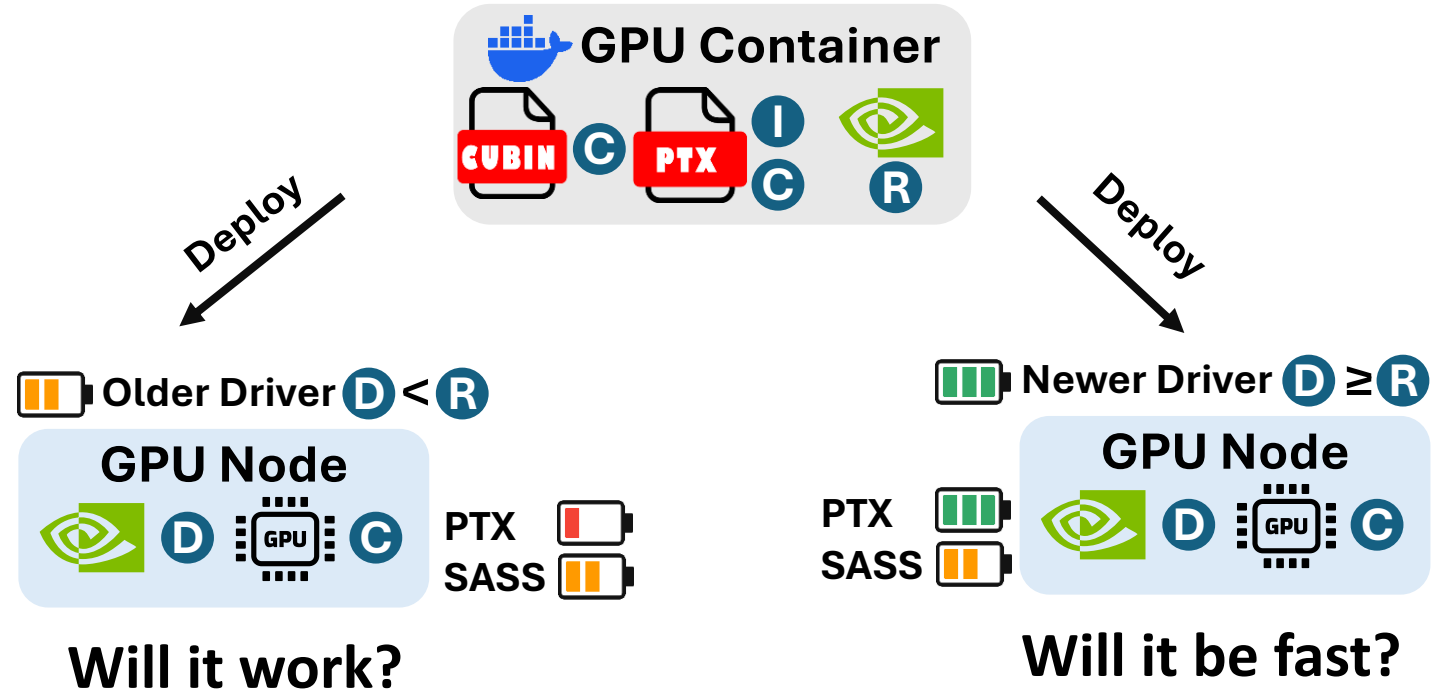
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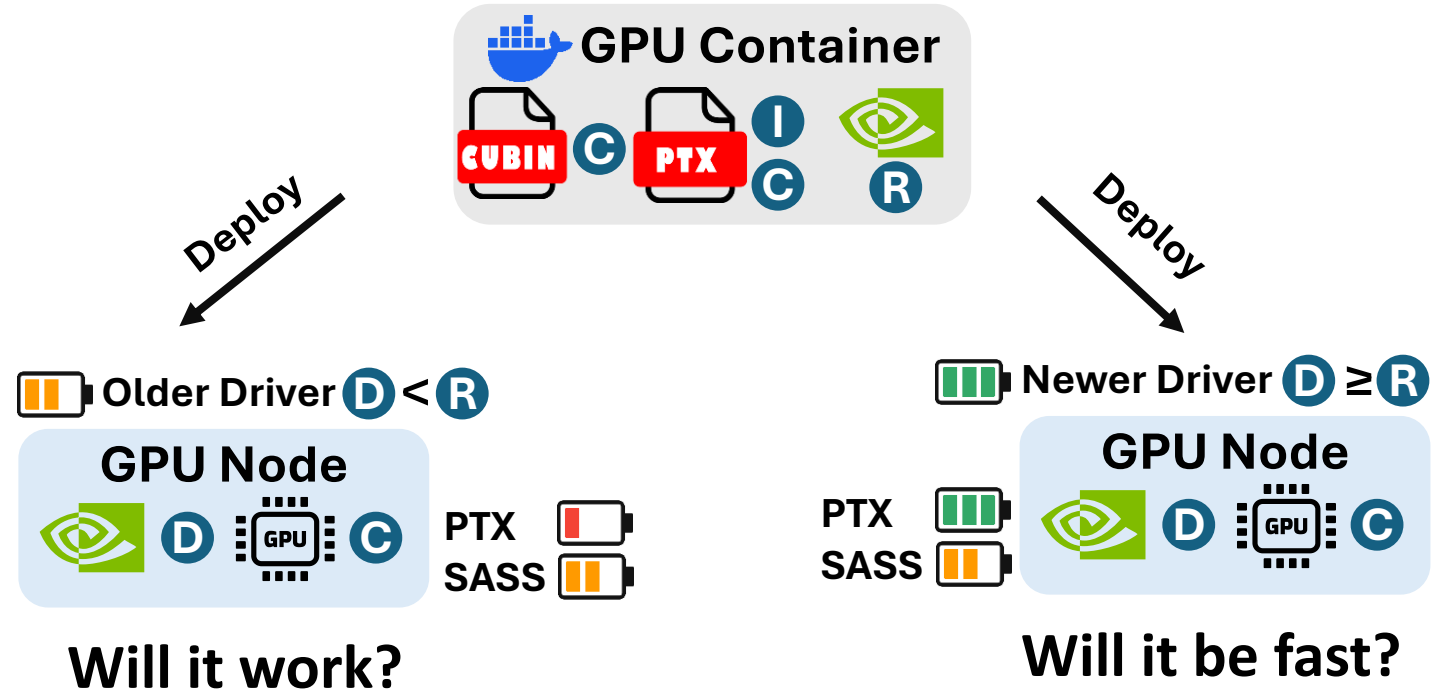


- ✔ Generate SASS for all supported versions + PTX for the highest version.

XaaS IR Containers: GPU Acceleration

CUDA Compatibility Model

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- ✔ Generate SASS for all supported versions + PTX for the highest version.
- ✔ Check for dependency on CUDA version.

Evaluation – Specialization Point Detection with LLMs



Prompt with Examples
(In-Context Learning)



JSON Schema



CMake Build Configuration

Evaluation – Specialization Point Detection with LLMs



Prompt with Examples
(In-Context Learning)
JSON Schema



Sample LLM
10 times.



CMake Build Configuration

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Prompt with Examples
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Sample LLM
10 times.



LLM Result

versus



Ground Truth

HPC Specialization Points

 CMake Build Configuration

Evaluation – Specialization Point Detection with LLMs



Prompt with Examples
(In-Context Learning)
JSON Schema



Sample LLM
10 times.



LLM Result

versus



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HPC Specialization Points

 CMake Build Configuration



ICL Test Case: GROMACS



Gemini 1.5 & 2.0
F1 Scores: 0.86 – 0.99

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HPC Specialization Points

 Prompt with Examples
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 JSON Schema



Sample LLM
10 times.



 LLM Result

versus

 Ground Truth

 CMake Build Configuration

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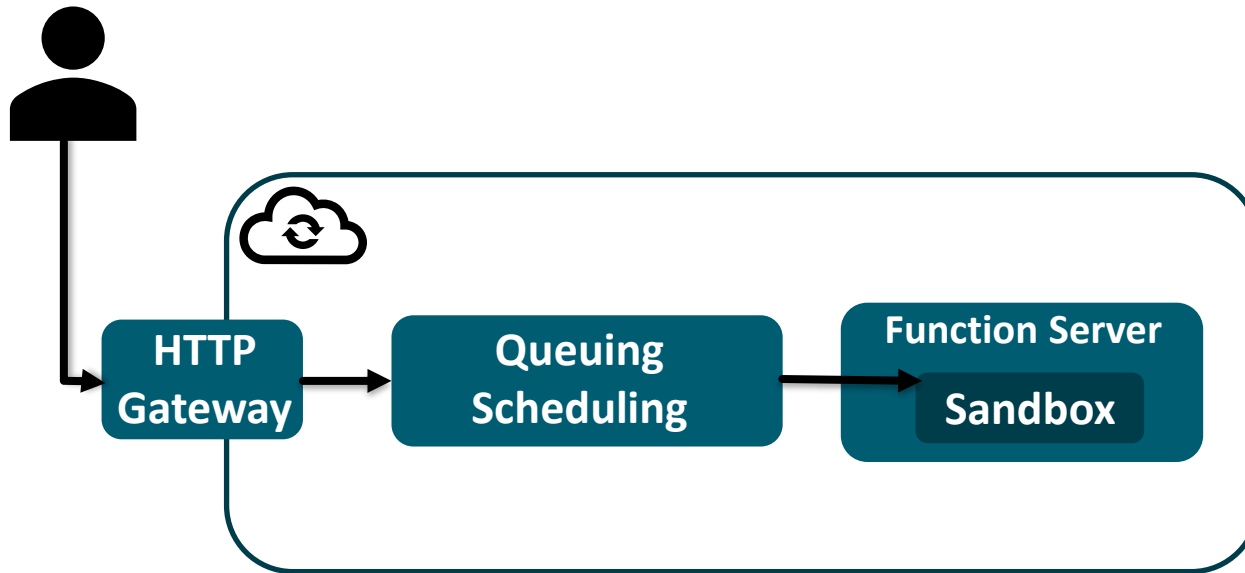
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F1 Scores: 0.86 – 0.99

Generalization: llama.cpp

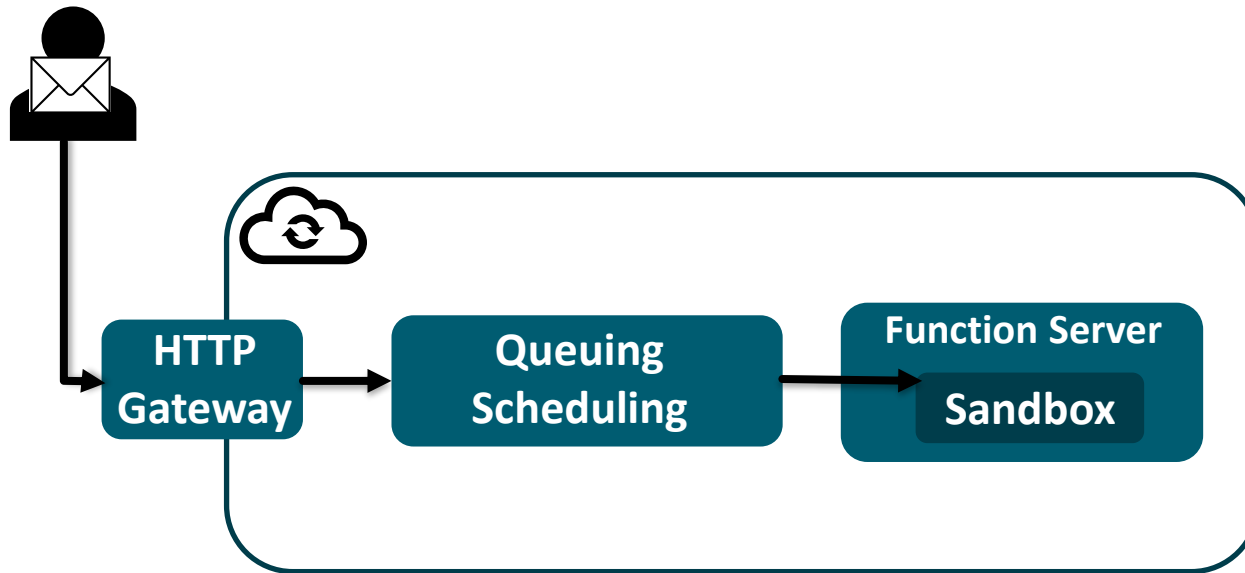


GPT-o3
F1 Scores: 0.73 - 0.79

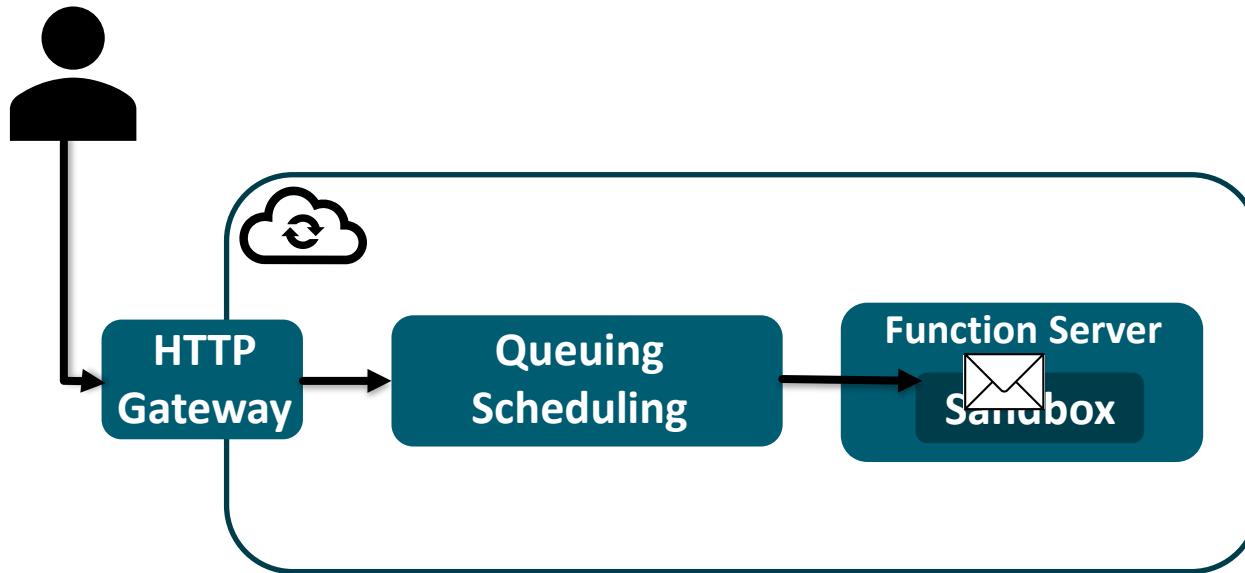
How does FaaS work?



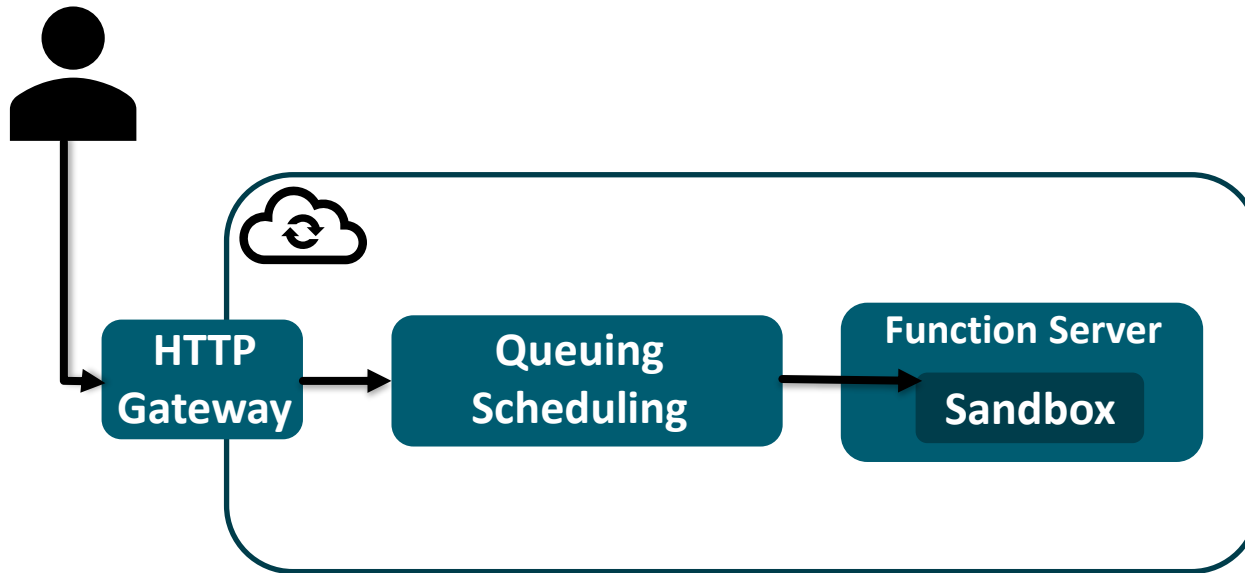
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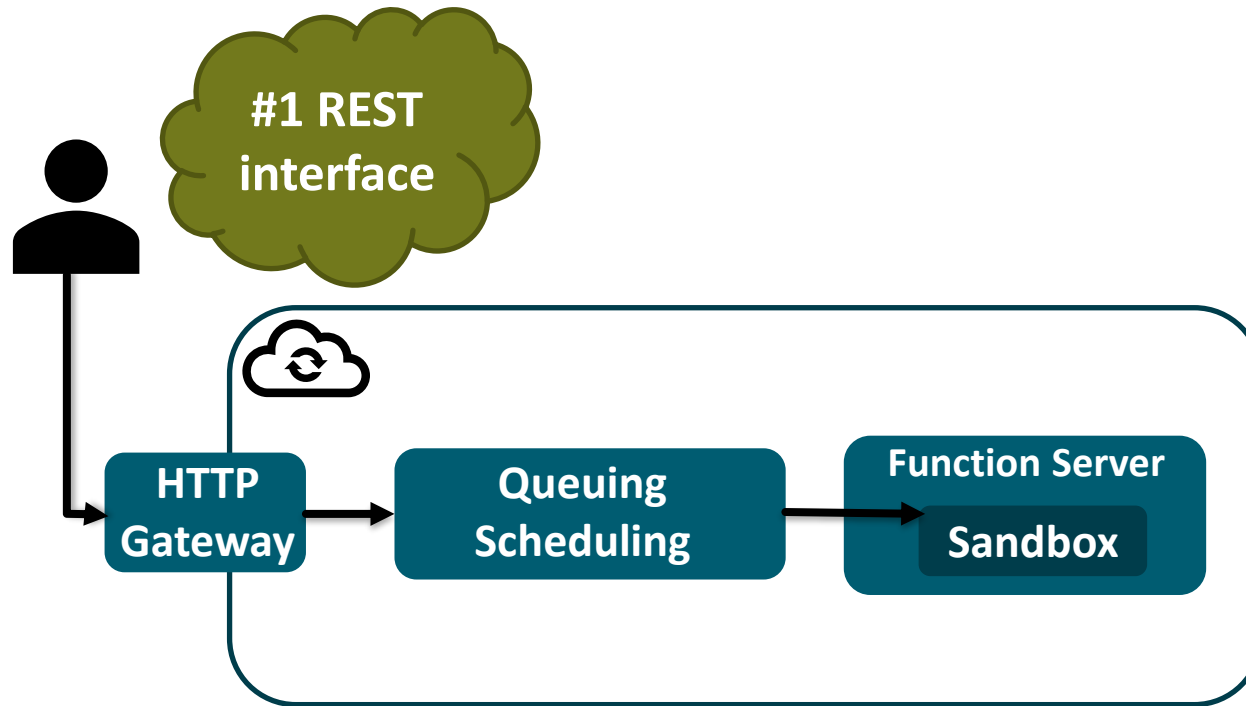
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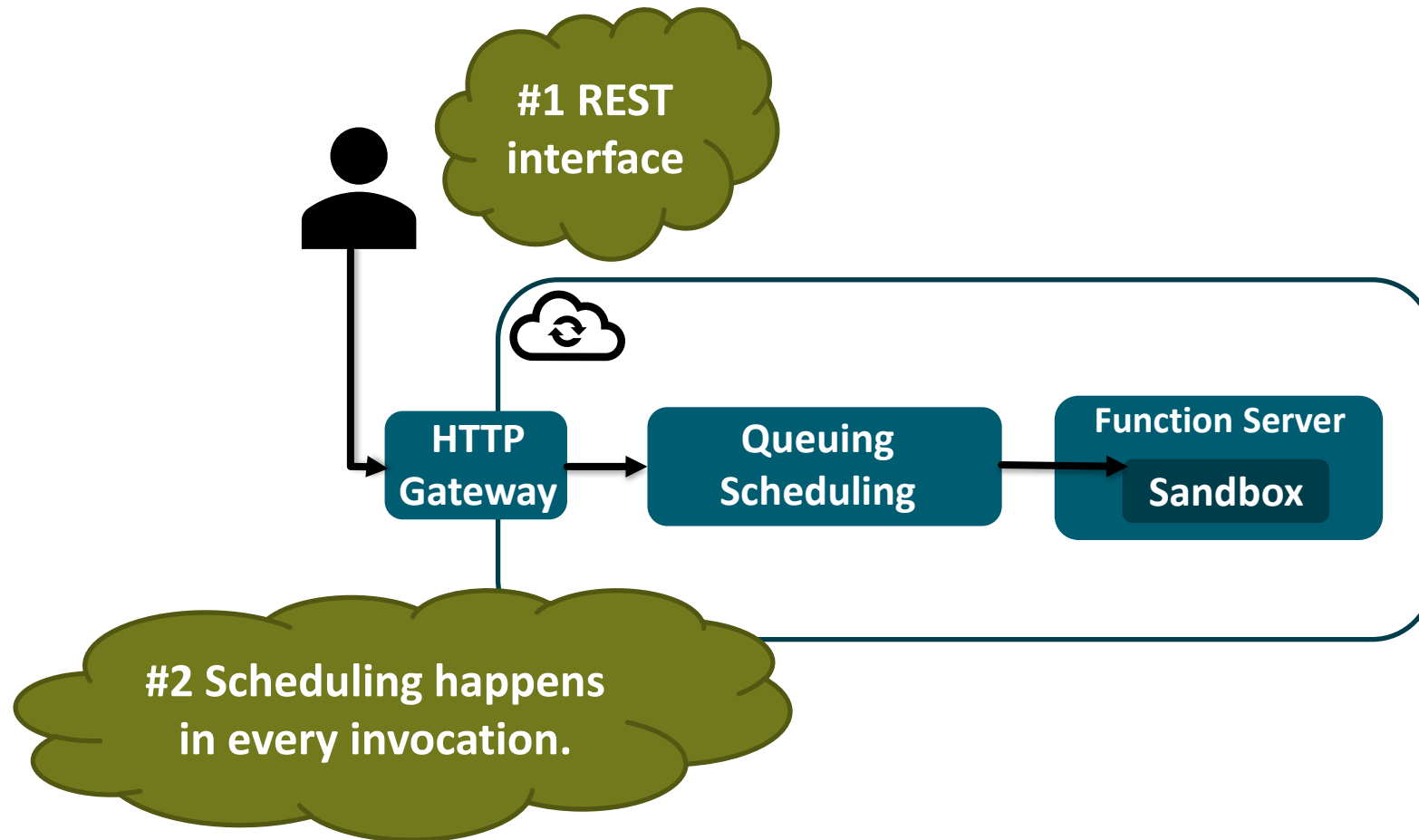
Why is FaaS slow?



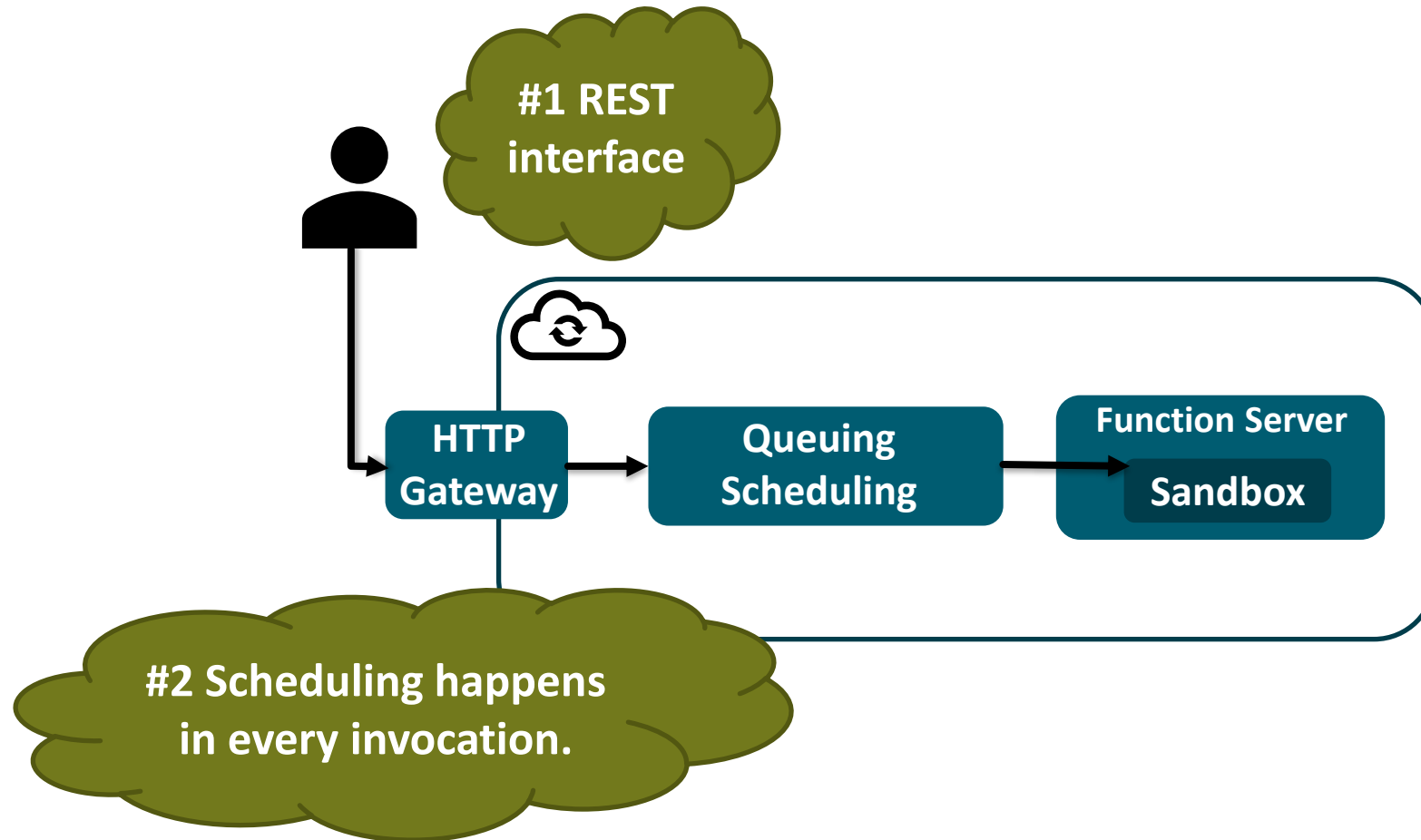
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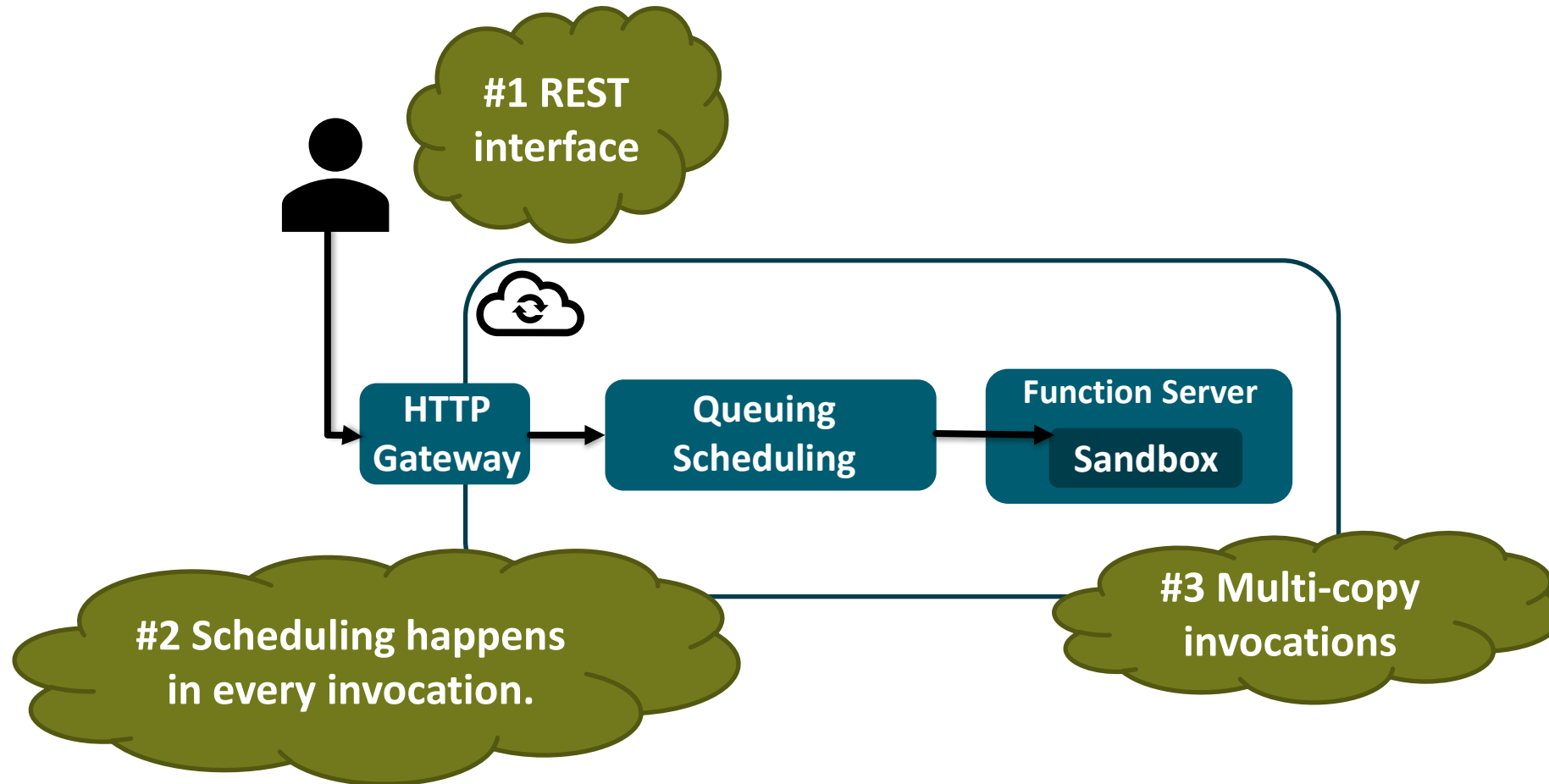
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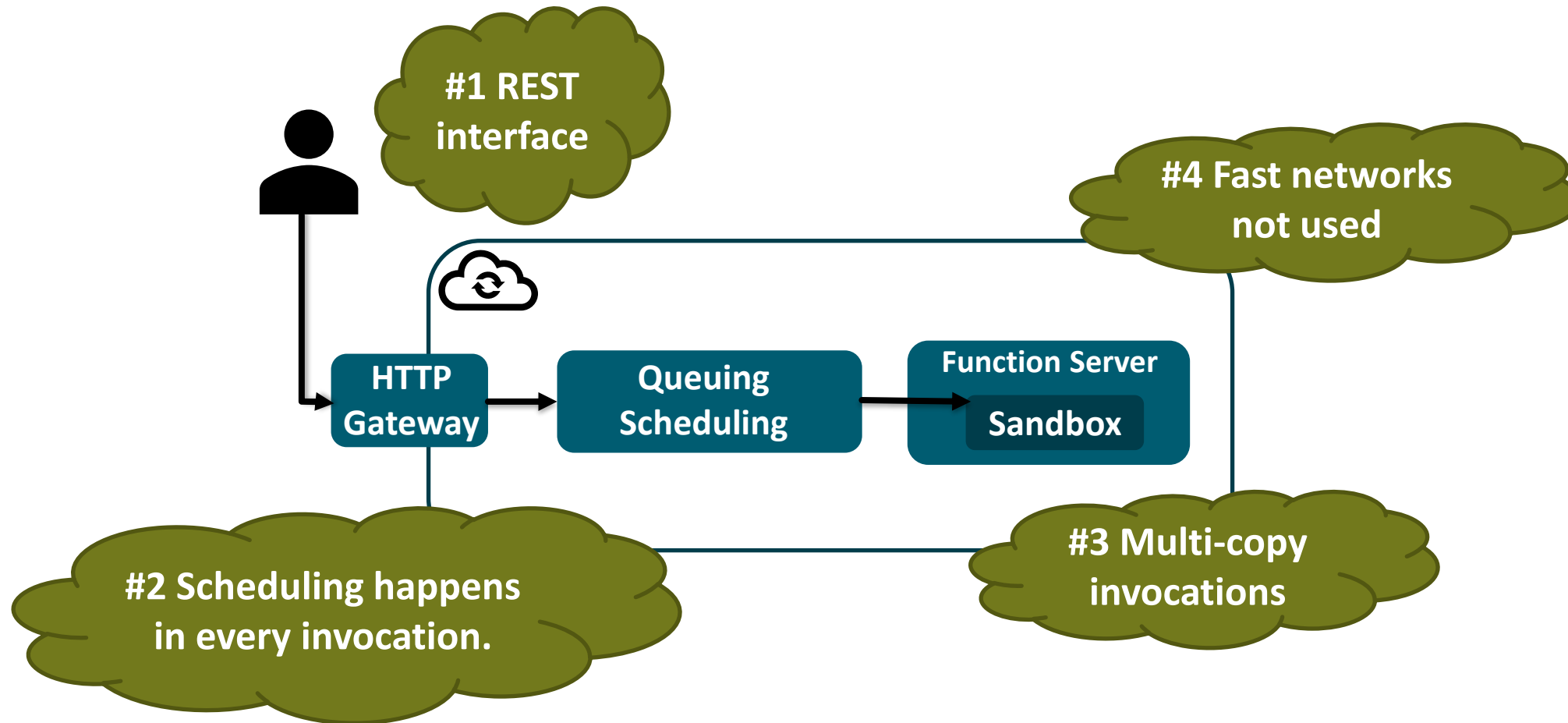
Why is FaaS slow?



“SeBS: a Serverless Benchmark Suite
 for Function-as-a-Service Computing”



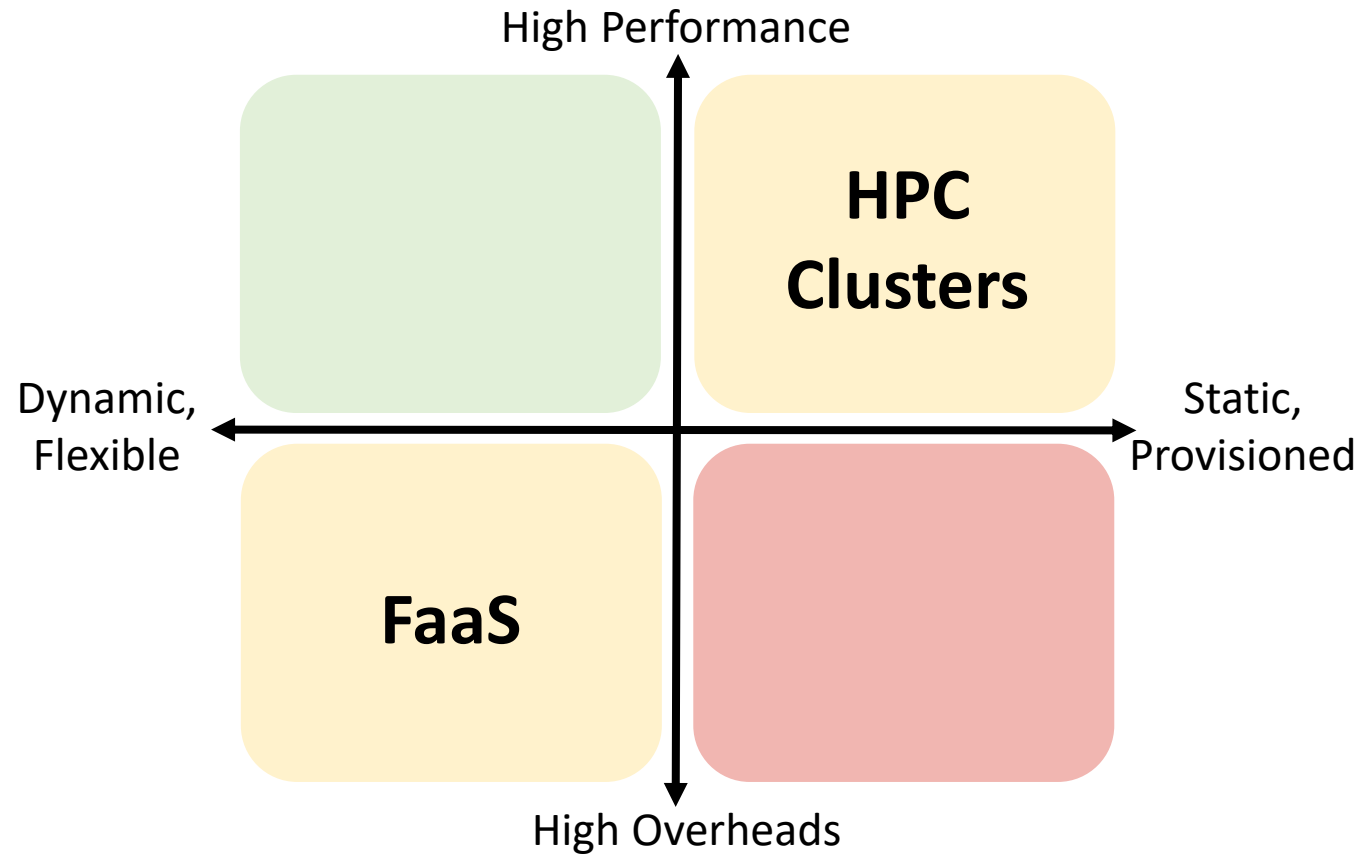
Why is FaaS slow?



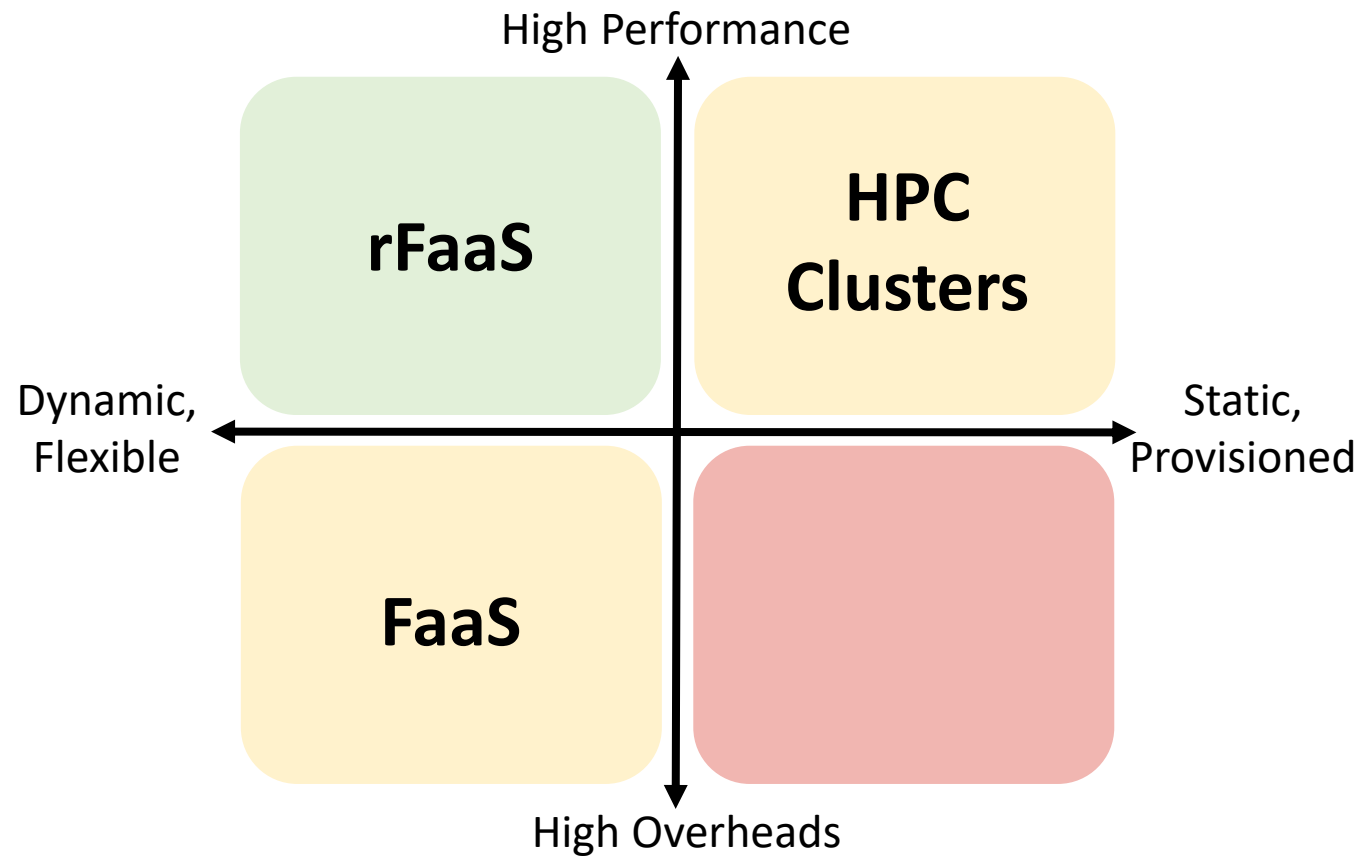
“SeBS: a Serverless Benchmark Suite
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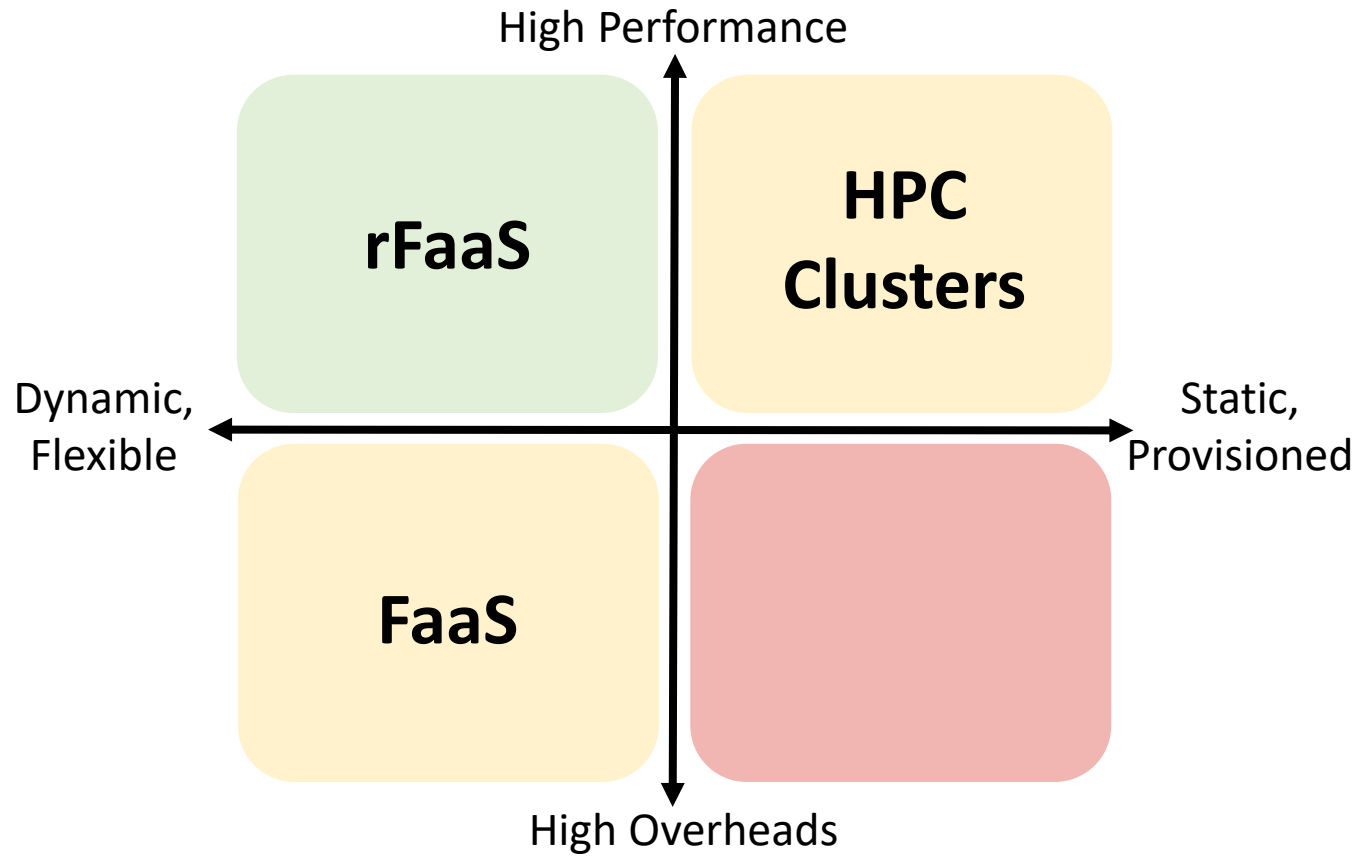
Function-as-a-Service for HPC



Function-as-a-Service for HPC



Function-as-a-Service for HPC

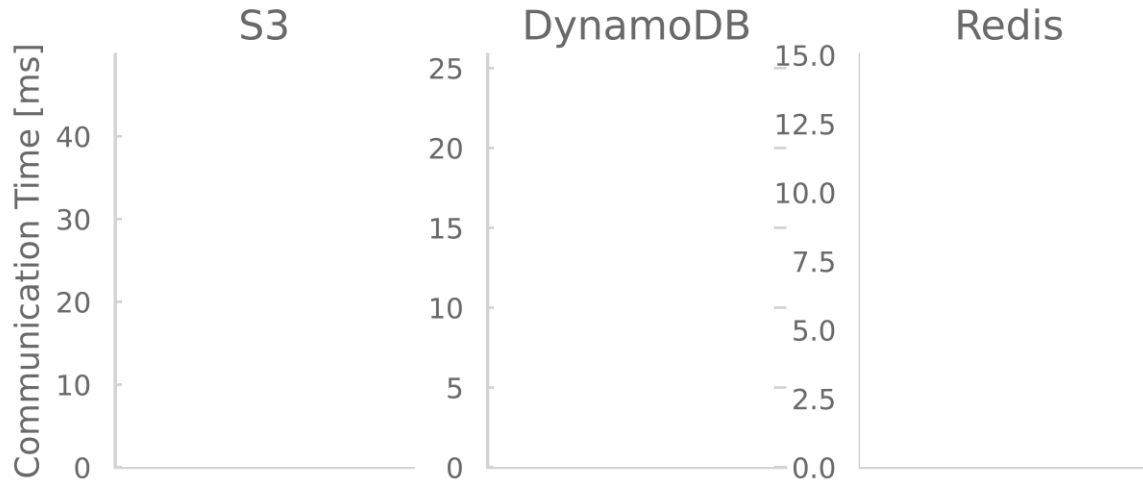


Reduced invocation critical path

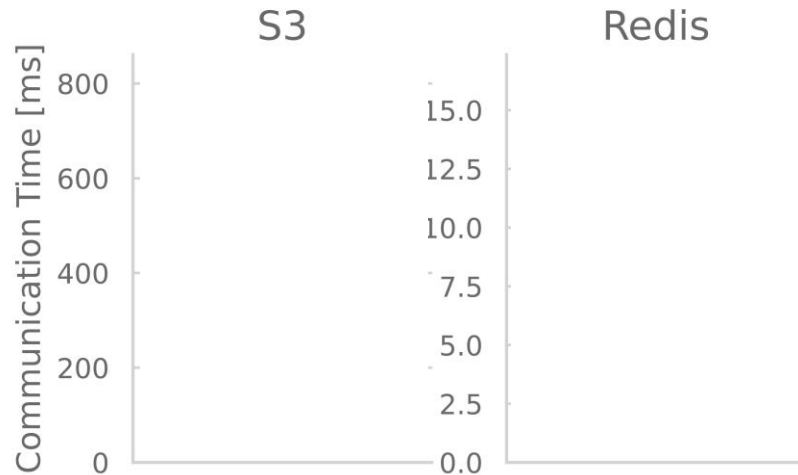
Zero-copy RDMA

Serverless Applications: Communication

1 B

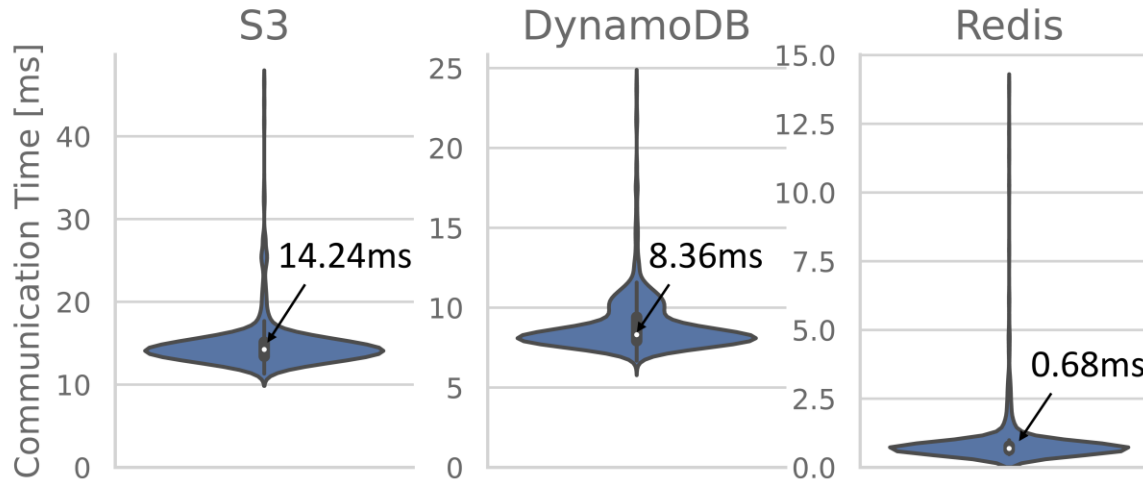


1 MB



Serverless Applications: Communication

1 B



1 MB

