Enabling HPC software productivity with the TAU performance system

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Outline

Two main parts, theory and then practice.

- **9:00 - 10:00: Enabling HPC software productivity with the TAU performance system**
  - A discussion on the role of performance tools in HPC
  - General outline of monitoring techniques and principles
  - A practical tour of the TAU performance system (features / how to)
- **10:30 - 11:45: Hands-on Session**
  - Deploy TAU
  - Profile real code
  - Look at various instrumentation techniques

Enabling HPC software productivity with the TAU performance system

Introduction

On Performance in…

High
Performance
Computing

Introduction

What is performance in the end ?

- **#1** Solving challenging problems with computing resources:
  - Domain specific knowledge (physicists, numericians, …)
  - Produce invaluable simulation results by solving **large** problems (requiring distributed memory and scale)
- **#2** Taking advantage of the latest hardware:
  - Using it **productively** to fulfill **#1** in a tight loop
  - Consider new techniques and models thanks to computing power (3D, ab-initio, higher-resolutions, …)

Introduction

Mind the gap

- **HPC is subject to the knowledge gap**
  - It is a field full of experts in their various domains
  - It is crucial to acknowledge that cross-disciplinary collaboration is needed
- **A numerician is not (always) a computer scientist:**
  - Mastering simulation (or other domain specific applications) and low-level programming (runtimes, architectures) is increasingly difficult
  - HPC is suffering from lack of abstractions between the computational layers (compute and runtime)

Introduction

On the surprising nature of HPC

- **HPC is a field of constant challenges…**
  - Cutting edge hardware every 2 years
  - Evolving runtime abstractions
- **And surprising stability …**
  - Large (multimillions lines) applications to port
  - A lot of Fortran, C and C++
  - Mostly (up to recently) MPI and OpenMP
    - MPI (mostly) backward compatible for 25+ years !

BUT

Things may change …

LLM

Large Language Models

ML now drives High-End Computing

Both fields are now bound to converge

- **GPUs are the core vector for LLMs**
  - Multi-Billion dollar market (for sure larger than HPC).
- **AI/ML payloads come with different programming habits**
  - Multi-language (not only native ones) -> PyTorch (Python + CUDA)
  - Generally easy to deploy (pip, cargo, docker)
  - Cloud-aware
- **And HPC will transitively benefit from those**


Interesting times ahead…

Making a Productive HPC Application

Choose and dose your priorities

- **Fulfilling the initial goal of the program**
  - Generate valuable domain-specific results
  - Achieve the desired resolution/throughput
- **Efficient use of the machine**
  - Do not waste computing power (vectorized, GPUs, CPUs, …)
  - Run **efficiently** at scale (do you really need these cores ?)
- **Maintainable code**
  - Keep the code easy to write and to read
  - Document the code avoiding cryptic parts
  - Write tests (for both performance and functionalities)

Optimizing too much is a mistake

AKA Leave AVX512 to the compiler as ..

Runtimes and Hardware are less uniform

The challenge is now impacting applications (not only runtimes)

- **Up to recently parallelism was « simple » (MPI and OpenMP, namely MPI+X)**
  - Using MPI for distributed memory
  - OpenMP for shared-memory programming
- **GPUs added another layer (+X+Y)**
  - Need to coordinate differentiated local memory regions
  - Need to handle more complex program states (nested computation)
- **And the world is less uniform…**
  - Keep the code easy to write and to read
  - Cuda, HIP, OpenACC, OpenMP (+Targets)
  - With little abstractions: Kokkos (C++)

Consider Following Agile Methods

Prepare for change and cope with it

- **You will have a broader set of languages to choose..**
  - C, Fortran, C++
  - Python (+ GPU)
  - Rust, Julia
- **A runtime..**
  - For distributed memory (in HPC MPI is dominating), other such as Mercury are appearing
  - For shared-memory (OpenMP, Threads, task oriented languages (async))
  - For your GPU (OpenMP Targets, Intel, AMD, Nvidia, …)
- **It means ..**
  - Rewriting code is now a necessary process when retargeting
  - The value of the program is not only in the code (also in algorithms, file-formats, doc, toolchain)
  - We are entering a multi-language era for HPC
  - **You need to be ready to assess the performance and operation of your code in many configurations**

MPI Forum is working on an ABI

Facilitating (among others) the use of MPI with other languages

MPI Application Binary Interface Standardization

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To be presented in September at EuroMPI 23.

Not Optimizing is also a mistake

You need to have performance as a fitting function.

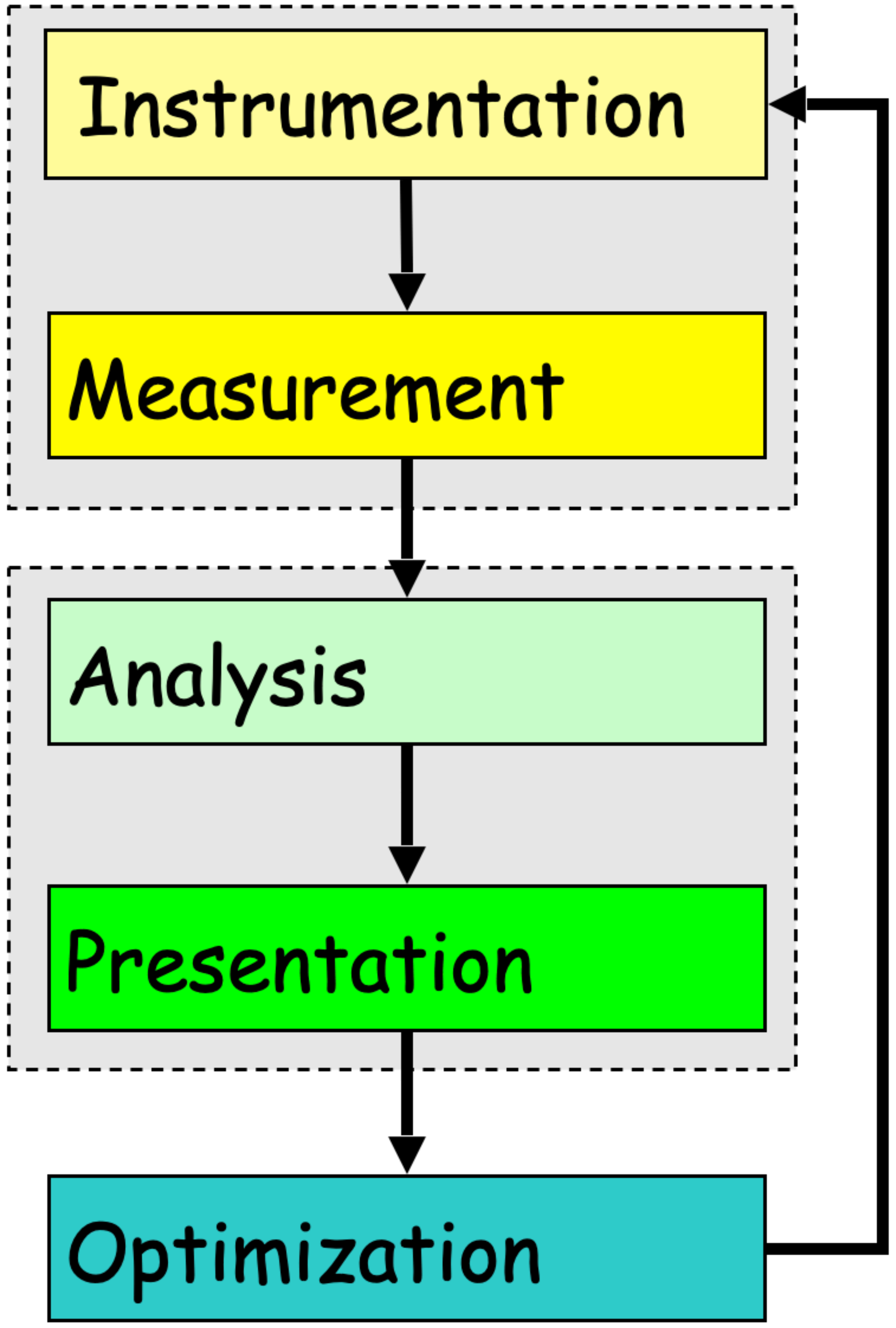
Performance Awareness

Make sure to track performance

- **Embed simple performance measurement metrics in your codes**
  - Simple counters testifying of the throughput
  - They should be domain specific and ideally language agnostic
- **Make your program modular**
  - Allows cross-language comparison
  - Forces separation of concerns
  - Enables plug & play replacement of some parts (for comparison)
- **Include performance measurement in your processes**
  - Automate in the CI (performance regression)
  - Include performance assessment in releases

Performance Optimization Cycle

- Expose factors
- Collect performance data
- Calculate metrics
- Analyze results
- Visualize results
- Identify problems
- Tune performance



TAU

Tuning and Analysis Utility

Performance Optimization Cycle

- **Tuning and Analysis Utilities (20+ year project)**
- **Comprehensive performance profiling and tracing**
  - Integrated, scalable, flexible, portable
  - Targets all parallel programming/execution paradigms
- **Integrated performance toolkit**
  - Instrumentation, measurement, analysis, visualization
  - Widely-ported performance profiling / tracing system
  - Performance data management and data mining
  - Open source (BSD-style license)
- **Integrates with application frameworks**

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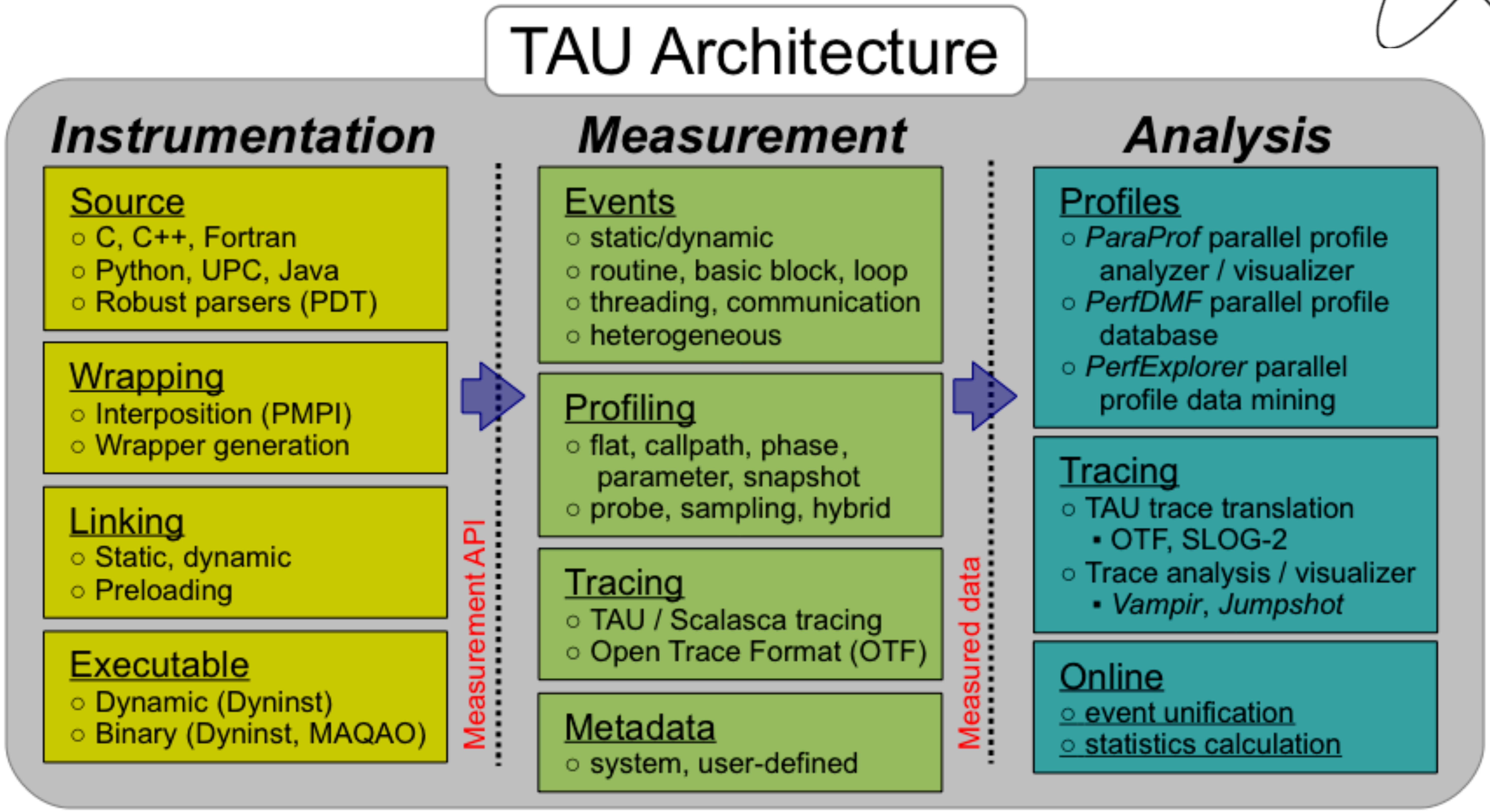
ParaTools

Understanding Application Performance using TAU

- How much time is spent in each application routine and outer *loops*? Within loops, what is the contribution of each *statement*?
- How many instructions are executed in these code regions?
  Floating point, Level 1 and 2 *data cache misses*, hits, branches taken?
- What is the memory usage of the code? When and where is memory allocated/de-allocated? Are there any memory leaks?
- What are the I/O characteristics of the code? What is the peak read and write *bandwidth* of individual calls, total volume?
- What is the contribution of each *phase* of the program? What is the time wasted/spent waiting for collectives, and I/O operations in Initialization, Computation, I/O phases?
- How does the application *scale*? What is the efficiency, runtime breakdown of performance across different core counts?

TAU Architecture and Workflow



TAU Architecture and Workflow

Instrumentation: Add probes to perform measurements
- Source code instrumentation using pre-processors and compiler scripts
- Wrapping external libraries (I/O, MPI, Memory, CUDA, OpenCL, pthread)
- Rewriting the binary executable

Measurement: Profiling or tracing using various metrics
- Direct instrumentation (Interval events measure exclusive or inclusive duration)
- Indirect instrumentation (Sampling measures statement level contribution)
- Throttling and runtime control of low-level events that execute frequently
- Per-thread storage of performance data
- Interface with external packages (e.g. PAPI hw performance counter library)

Analysis: Visualization of profiles and traces
- 3D visualization of profile data in paraprof or perfexplorer tools
- Trace conversion & display in external visualizers (Vampir, Jumpshot, ParaVer)