Identifying Performance Bottlenecks in Hybrid MPI + OpenMP Software

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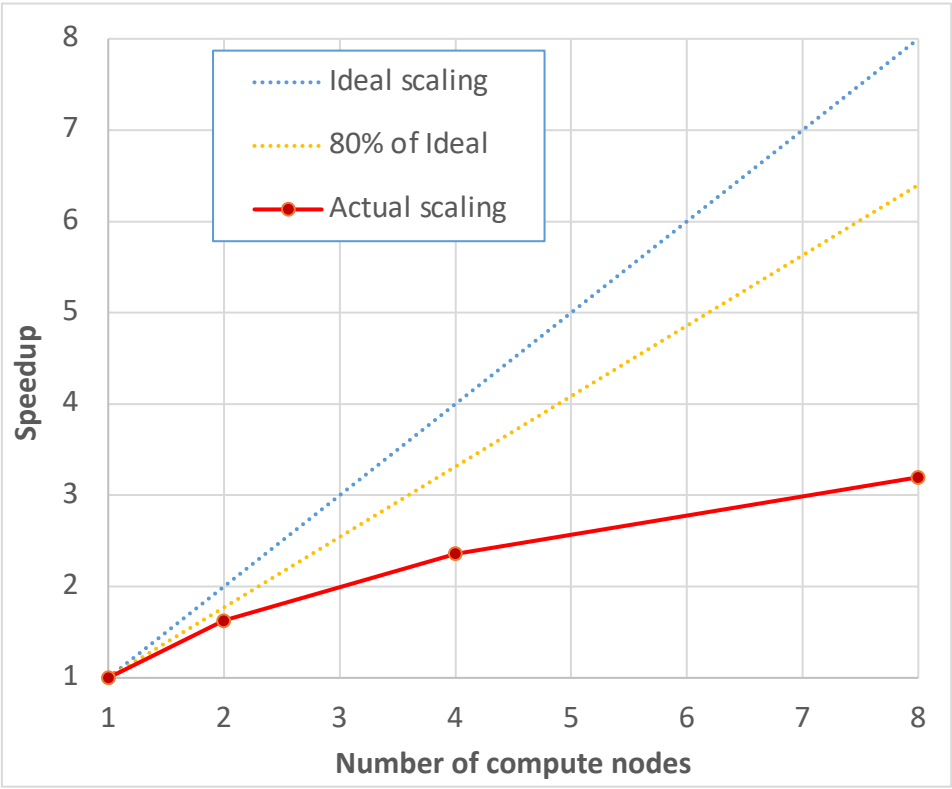
The problem we're addressing

- Getting good parallel performance is hard!!!
- Even with the simplest parallelism we need to think about
  - Serialisation
  - Load balance
  - Memory bottlenecks
  - Processor frequency
  - Instruction count
  - Overheads of parallelization
- MPI + OpenMP adds complexity
  - Is the problem in the OpenMP?
  - Or the MPI?
- And parallel scaling tells us nothing about what is wrong!!



Performance analysis tools

- There are powerful tools to us help analyse performance
  - BSC toolset – Extrae, Paraver, Dimemas, etc
  - Scalasca toolset – Score-P, Scalasca, Cube
  - Intel's tools – VTune, ITAC, etc
  - Plus many more
- But the data they generate is often overwhelming
  - Extremely detailed and complex event timelines per thread
  - Vast amounts of difficult to understand metrics
- **We need to make sense of the trace data before we know what we're looking for in the trace data**
  - But how???

The solution – the POP metrics

- **An easy to understand set of metrics**
- **Metrics which can be easily calculated from typical trace data**
- **Metrics which point at specific causes of performance bottlenecks**

- This idea has been successfully demonstrated by POP's MPI metrics
- We now extend to hybrid MPI + OpenMP (& beyond?)
  - We have **two** approaches for hybrid, both based on the POP MPI metrics
- One extends the idea of defining an individual metric per source of inefficiency
- The other extends the multiplicative approach of the MPI metrics

POP's high level metrics

- The POP methodology defines hierarchies of metrics
  - See POP online training "*Understanding Application Performance with the POP Metrics*" for details
- The top level metrics for both MPI + OpenMP schemes are identical
  - And are the same as those in POP's MPI metrics

1. **Parallel Efficiency**
   - How efficient is the parallelisation?
2. **Computation Scaling**
   - Is the total useful computation increasing or decreasing?
3. **Global Efficiency**
   - Combines inefficiency from parallelisation and computation scaling

POP's high level metrics

- We measure ***comp*** = time in useful computation on each CPU core
  - i.e. the time spent executing useful user code
- And ***comp_ref*** = useful computation on a reference case
  - Usually the smallest number of cores used e.g. 1 compute node
- Assuming strong computation scaling:

Parallel Efficiency = average(*comp*) / *runtime*

Computation Scaling = sum(*comp_ref*) / sum(*comp*)

Global Efficiency = Computation Scaling x Parallel Efficiency

Hybrid metrics method 1

The POP ‘additive’ scheme for MPI + OpenMP

The idea of ‘additive’ metrics

- Lets revisit POP’s **Parallel Efficiency**
  - This measures the efficiency of the parallelisation
- We measure ***comp*** and ***runtime*** on ***n*** cores
  - ***comp*** is useful computation per CPU core

Parallel Efficiency = average(*comp*) / *runtime*

- We can think of **average(*comp*)** as an **ideal runtime**

Parallel Efficiency ideal runtime = average(*comp*) = sum(*comp*) / *n*

- It is the runtime we would get if all useful work (***comp***) is split evenly over the cores with no overheads from the parallelism

The idea……

- Now look again at POP's **Global Efficiency**
  - This measures efficiency of the parallelisation combined with inefficiency due to increases in useful computation
- ***comp_ref*** is useful computation on our reference case
- ***n*** is number of cores for other cases under consideration

Global Efficiency = [sum(*comp_ref*)/*n*] / *runtime*

- We can think of an 'ideal runtime' for Global Efficiency

Global Efficiency ideal runtime = sum(*comp_ref*)/*n*

- This is the runtime we would get if the work from the reference case was to be split evenly over ***n*** cores with no overheads

POP's 'additive' metrics

- Define performance bottlenecks that can be mapped to **known issues**
- For each class of performance bottleneck define an 'ideal runtime'
- Then for each class of bottleneck:

efficiency = ideal runtime / runtime

- We can also define:

inefficiency = 1 - efficiency

  - For optimal performance: efficiency = 1, and inefficiency = 0

- This defines a hierarchy where we can **add** 'child' inefficiency values to get the 'parent' inefficiency value
  - Since **inefficiency = 'time cost of bottleneck(s)' / runtime**
  - Splitting the cost of the bottleneck into the individual contributions is the same as splitting the inefficiency value

Additive metrics for MPI + OpenMP

- We start with Parallel Efficiency and want to split this into child metrics
- With additive metrics we have complete freedom about how we define child metrics

- One obvious option is to split Parallel Efficiency into
  1. Process Efficiency (ignores all thread inefficiencies)
  2. Thread Efficiency (ignores process inefficiencies)

Parallel Inefficiency = Process Inefficiency + Thread Inefficiency

Illustration: Process Efficiency

- To assess Process Efficiency we want to know
  1. How evenly ‘useful work’ is distributed over the processes
  2. How much time the processes spend in MPI

- If we ignore the threading there are only three states, i.e.
  1. A process is in serial computation on the master thread: ***serial_comp***
  2. A process is inside an OpenMP parallel region: ***omp***
  3. A process is inside MPI and outside OpenMP

- When ignoring the threading we assume only time outside OpenMP and inside MPI is non-useful

Illustration: Process Efficiency

- We define ***serial_comp*** and ***omp*** as useful
  - Time in MPI and outside OpenMP is considered the bottleneck

useful* = *serial_comp* + *omp

- And we can define an ‘ideal runtime’ as **average(*useful*)**

Process Efficiency = average(*useful*) / *runtime*

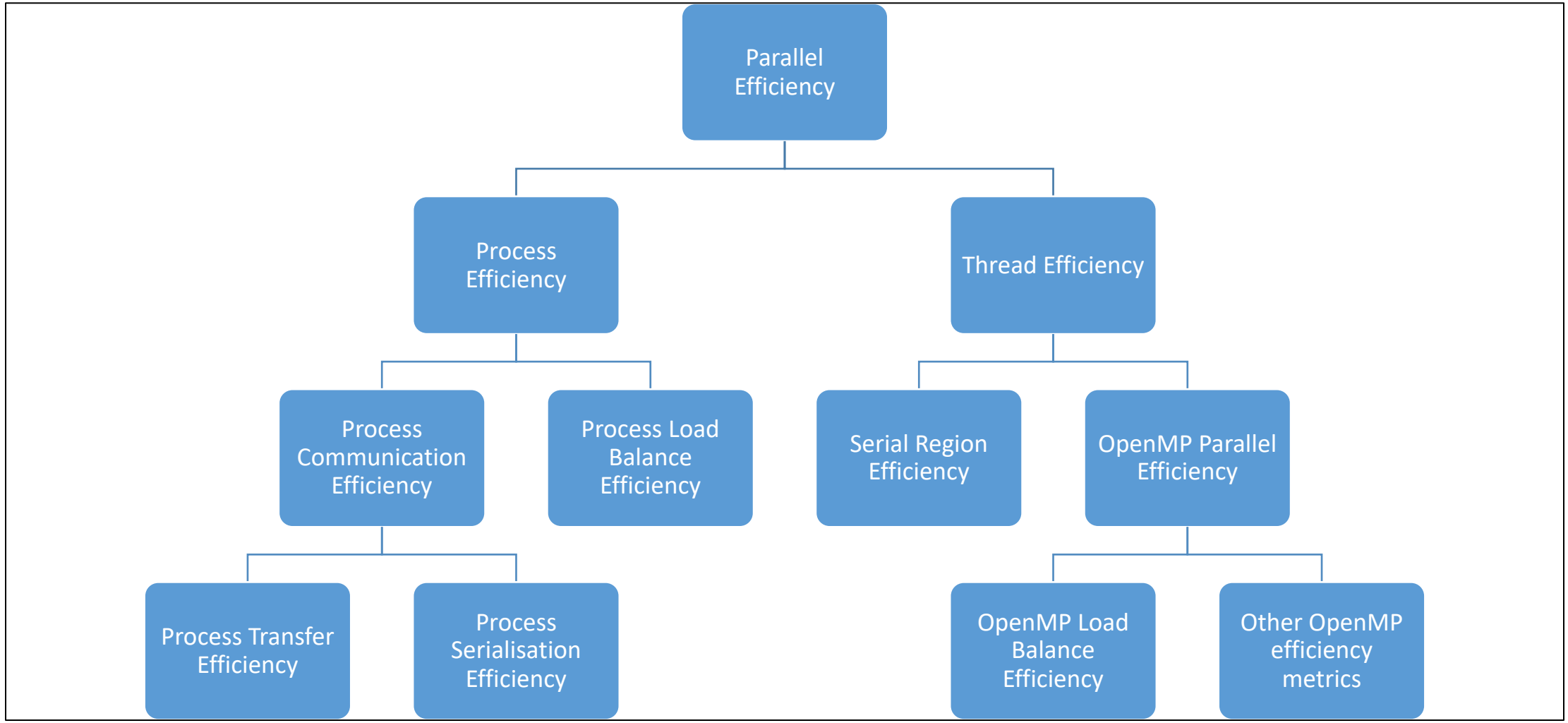
- We can use the additive methodology to define ideal run times that split Process Efficiency into
  - **Load Balance Efficiency** – cost of imbalance of ***useful*** over processes
  - **Transfer Efficiency** – cost of MPI time due to data transfer over network
  - **Serialisation Efficiency** – remaining cost of time in MPI

Thread Efficiencies

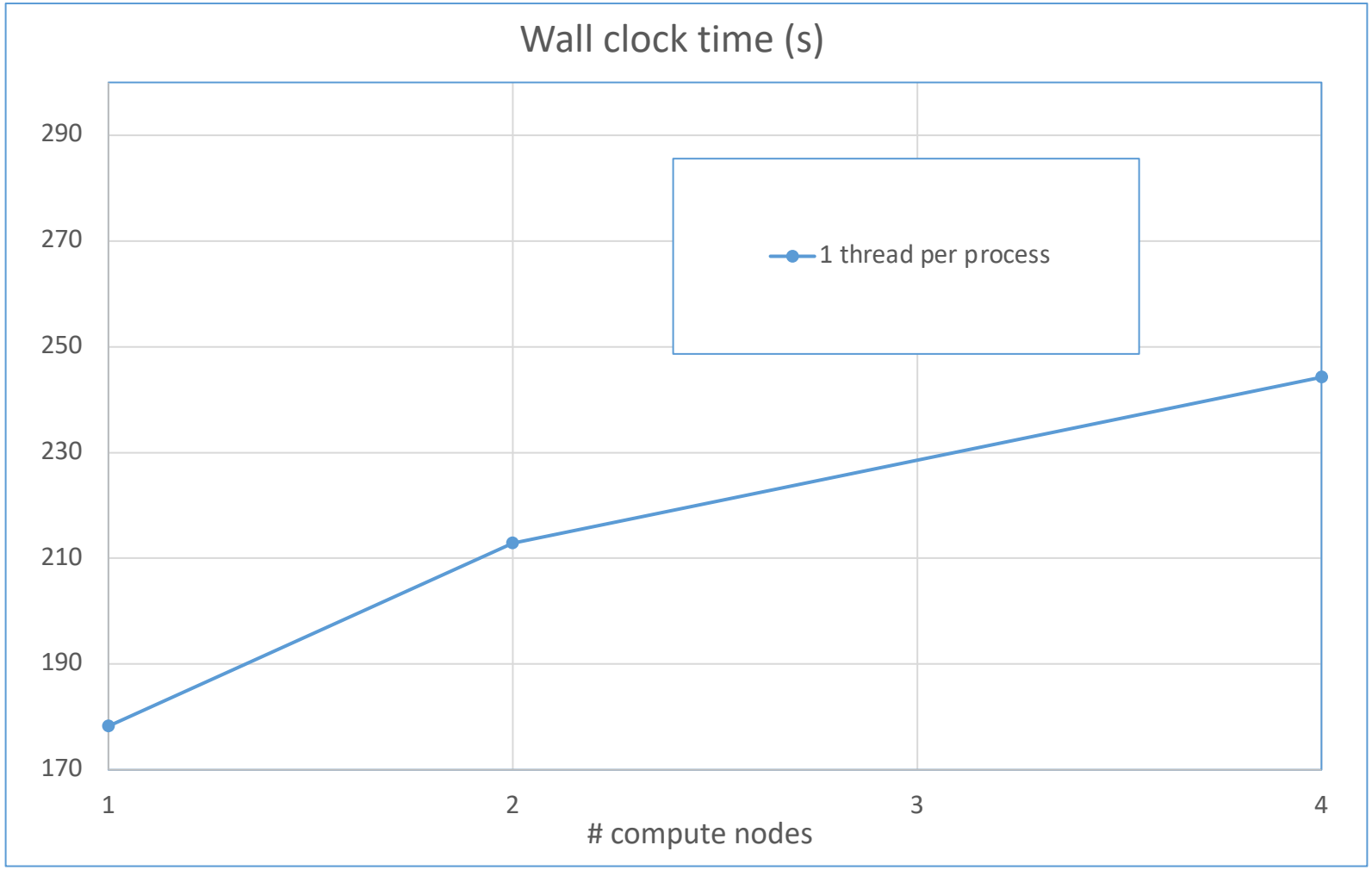
- We can define ideal runtimes which define
  - **Thread Efficiency** – cost of remaining non-useful time
  - Thread Efficiency sub metrics
    - **Serial Region Efficiency** – cost of computation outside OpenMP
    - **OpenMP Parallel Efficiency** – cost of time outside useful computation in OpenMP regions

- And we can also split OpenMP Parallel Efficiency e.g.
  - A contribution per OpenMP bottleneck
    - e.g. cost of thread load imbalance within OpenMP
  - Inefficiency contributions per OpenMP parallel region

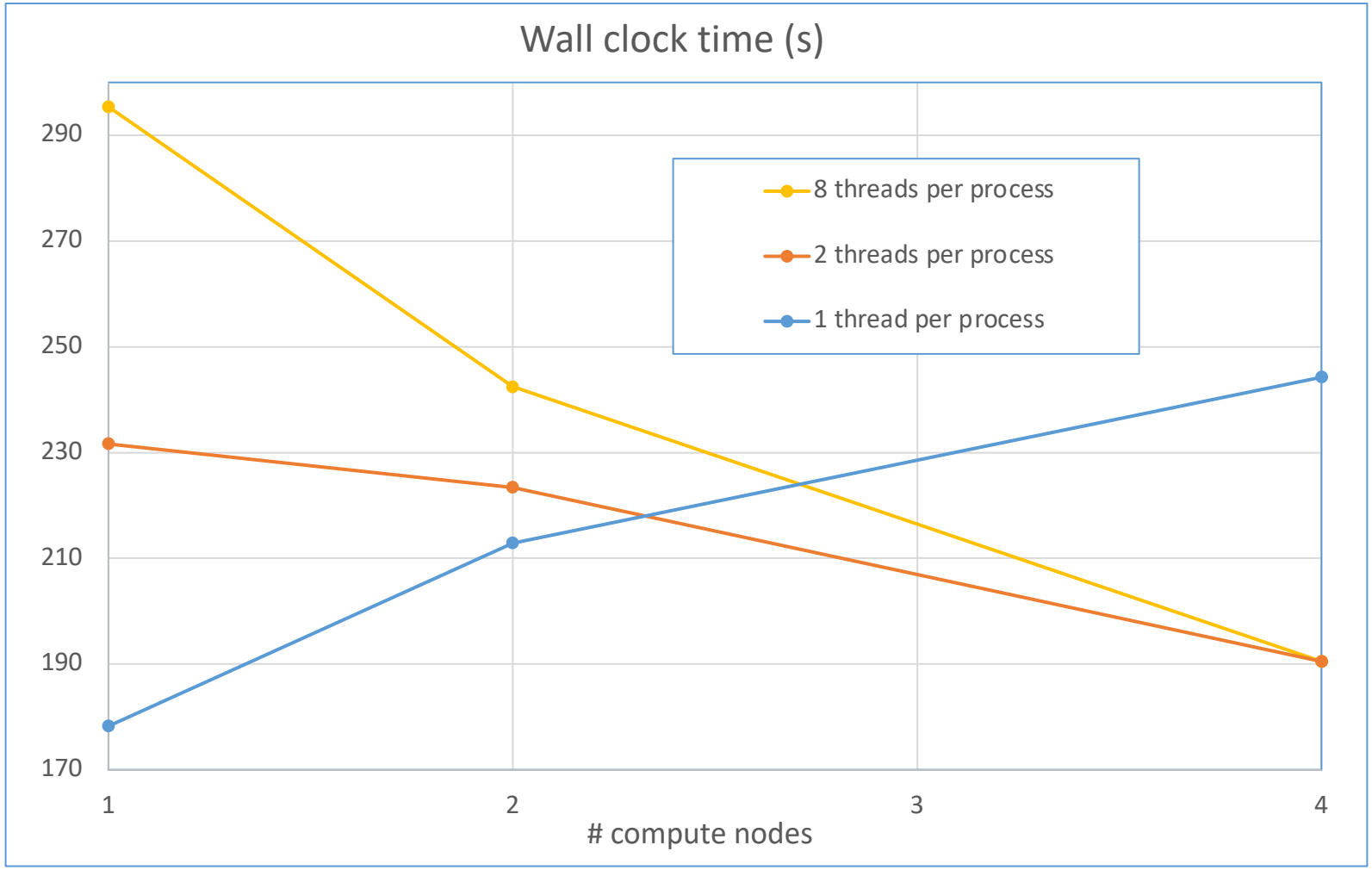
Additive metrics hierarchy



Example (strong scaling)



What is going on?



POP metrics to the rescue!

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What needs investigating further?

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Single thread issues

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Single node hybrid performance

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Single versus multiple node hybrid

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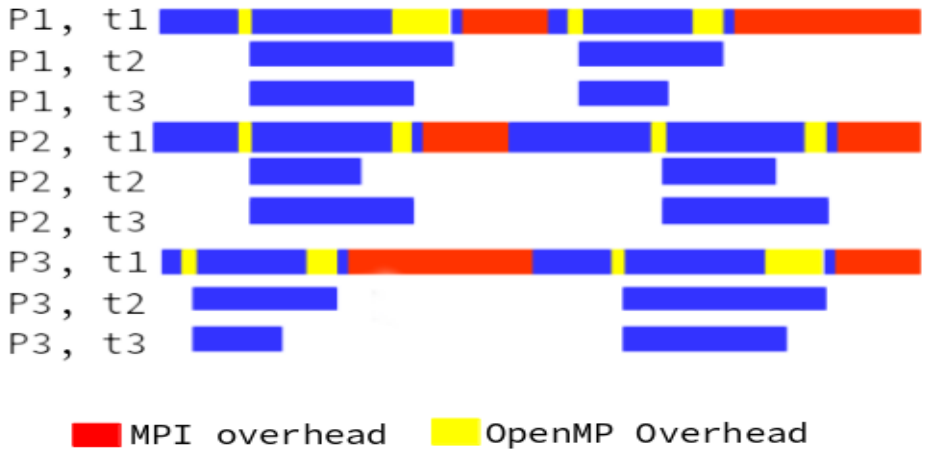
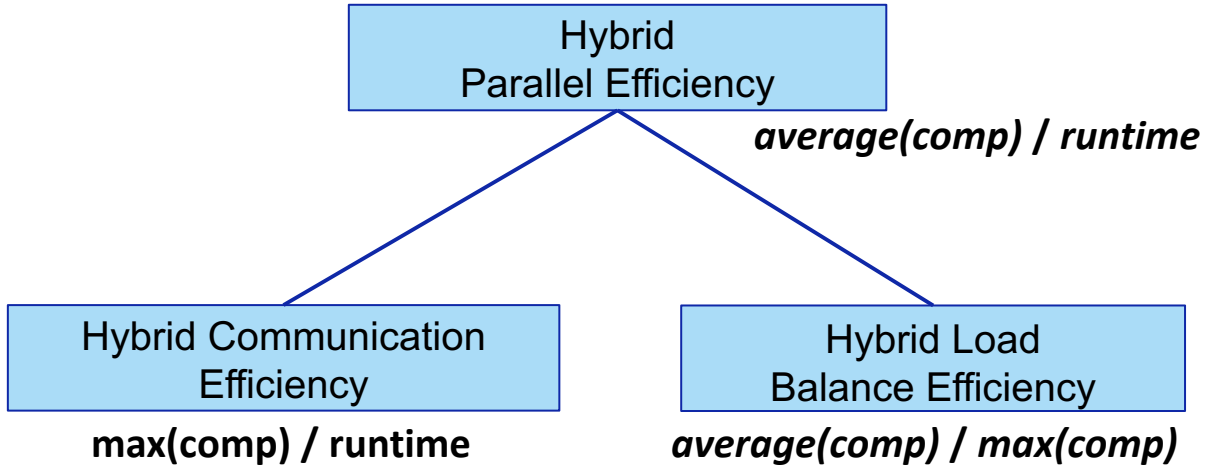
Hybrid metrics method 2

The POP ‘multiplicative’ scheme for MPI + OpenMP

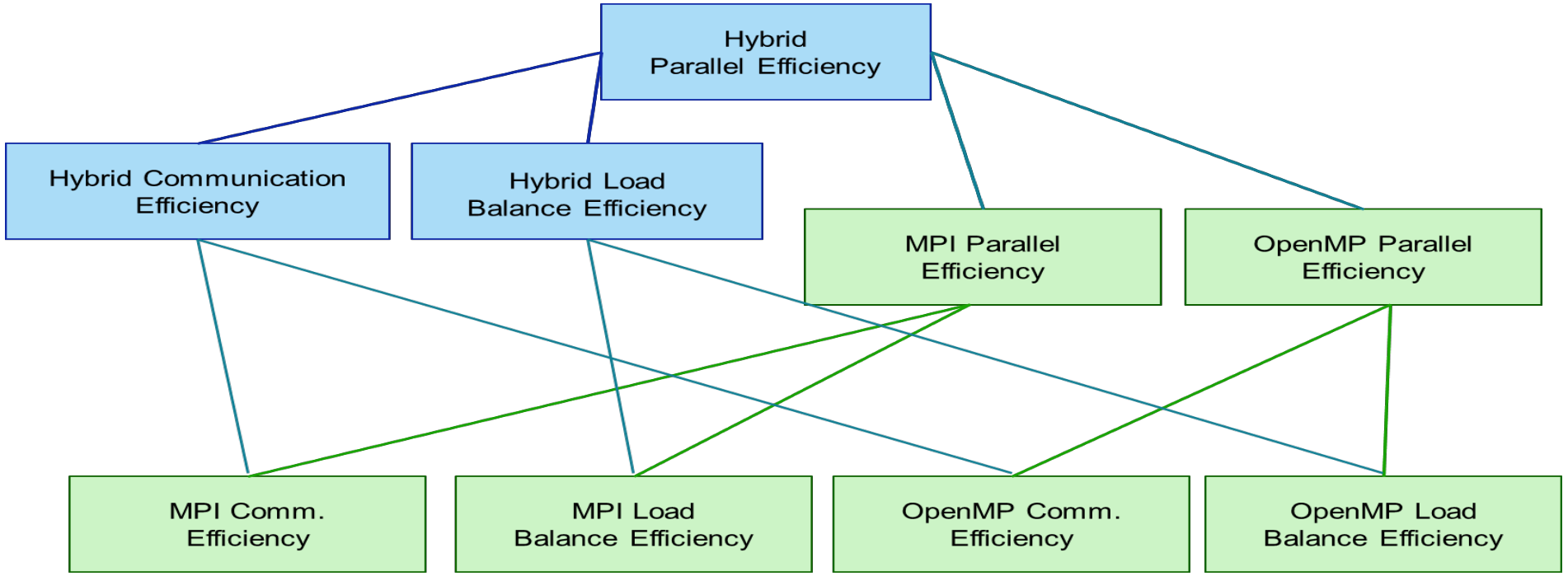
Applying the original model to hybrid codes





- Efficiency computed as percentage of time outside the two parallel runtimes
- Useful as a first step to distinguish between Load Balance and Communication. But how to dig down?
  - Efficiencies are mixing inefficiencies from MPI and OpenMP → Need to distribute the blame between the two programming models

What do we want?



- Global load balance and communication concepts can be mapped to any parallel programming paradigm
- The efficiencies at hybrid level collapse the contributions from the two programming models

Isolating MPI

- First target: hierarchical codes where MPI is the upper level (approach for 90% of the hybrid codes). From the MPI point of view, OpenMP runtime is as useful as computation:

MPI Parallel Efficiency = average*(out_MPI)* / *runtime*

Duration of the computing regions

Hybrid efficiencies [%]
- Parallel efficiency 47.07
- Load Balance 52.09
- Communication 90.37

MPI calls

MPI efficiencies [%]
- Parallel efficiency 95.97
- Load Balance 98.87
- Communication 97.06

OpenMP efficiencies

- Whatever cannot be blamed on MPI is caused by OpenMP. For example:

OpenMP Parallel Eff. = Hybrid Parallel Eff. / MPI Parallel Eff.

Duration of the computing regions

OpenMP efficiencies [%]

Parallel efficiency 49.05

Load Balance 52.69

Communication 93.11

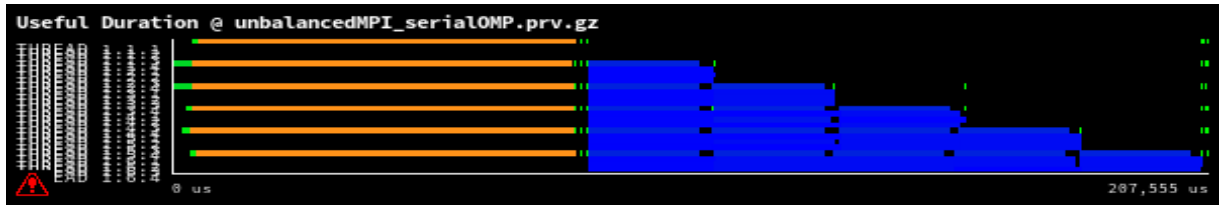
OpenMP parallel functions

→ The model is properly reporting that the main problem is imbalance in the OpenMP parallelization – large computation on the left only executed by the master thread.

Validating the source of imbalance

- Synthetic code with two very different phases

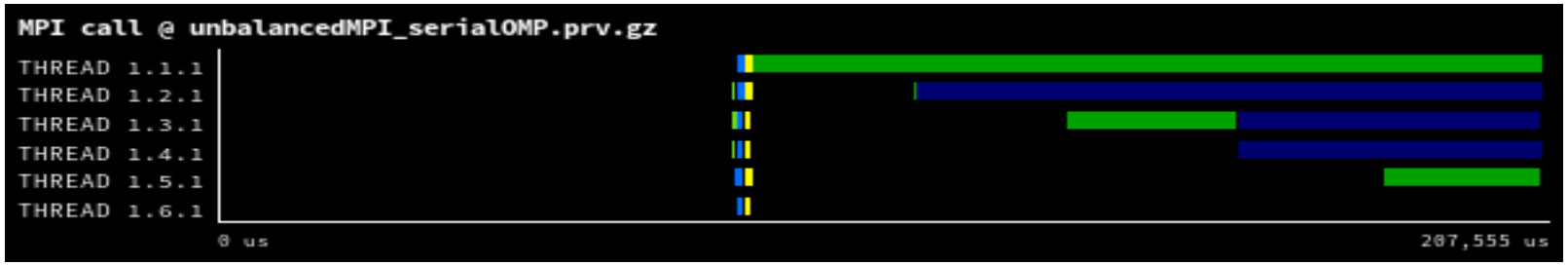
Duration of the computing regions



phase 1 *phase 2*

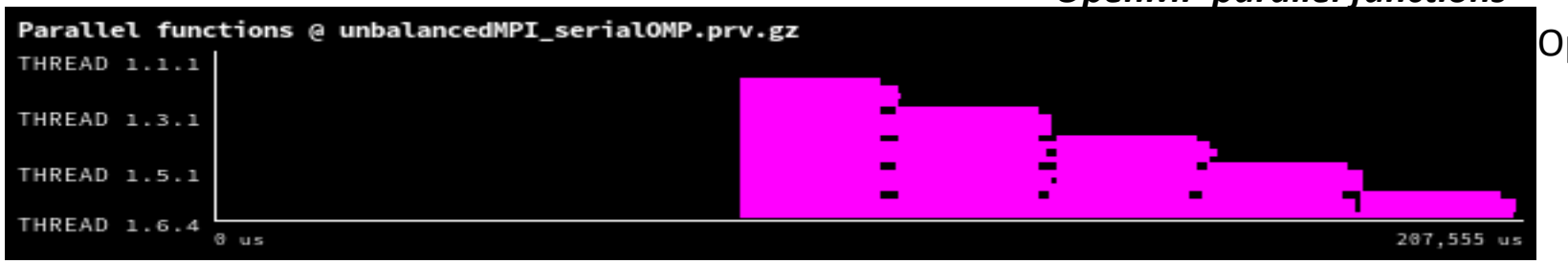
Hybrid efficiencies [%]
- Parallel efficiency 43.68
- Load Balance 48.46
- Communication 90.14

MPI calls



MPI efficiencies [%]
- Parallel efficiency 69.12
- Load Balance 70.01
- Communication 98.6

OpenMP parallel functions



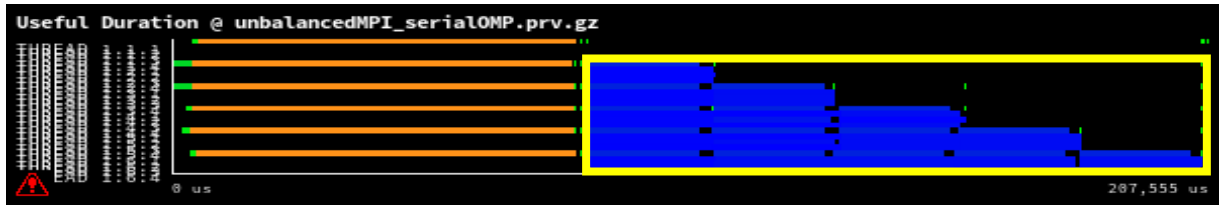
OpenMP efficiencies [%]
- Parallel efficiency 63.19
- Load Balance 69.22
- Communication 91.42

Phase 1 → OpenMP imbalance (previous slide), phase 2 → MPI imbalance?

Validating the source of imbalance

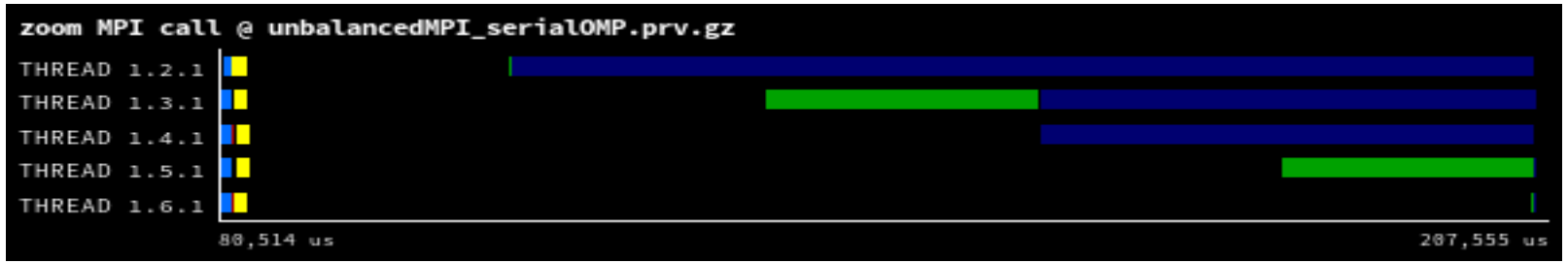
- Zooming in the second phase we can validate our guess

Duration of the computing regions



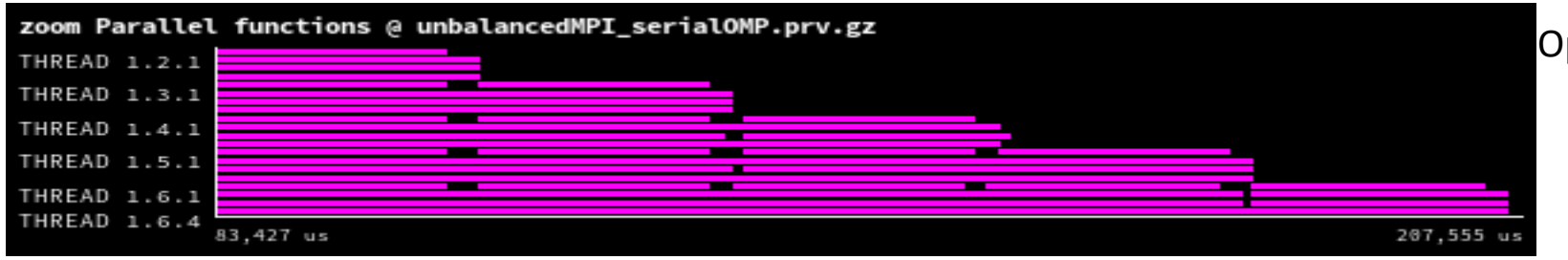
Hybrid efficiencies [%]
- Parallel efficiency 55.95
- Load Balance 58.78
- Communication 95.19

MPI calls



MPI efficiencies [%]
- Parallel efficiency 59.83
- Load Balance 61.20
- Communication 97.74

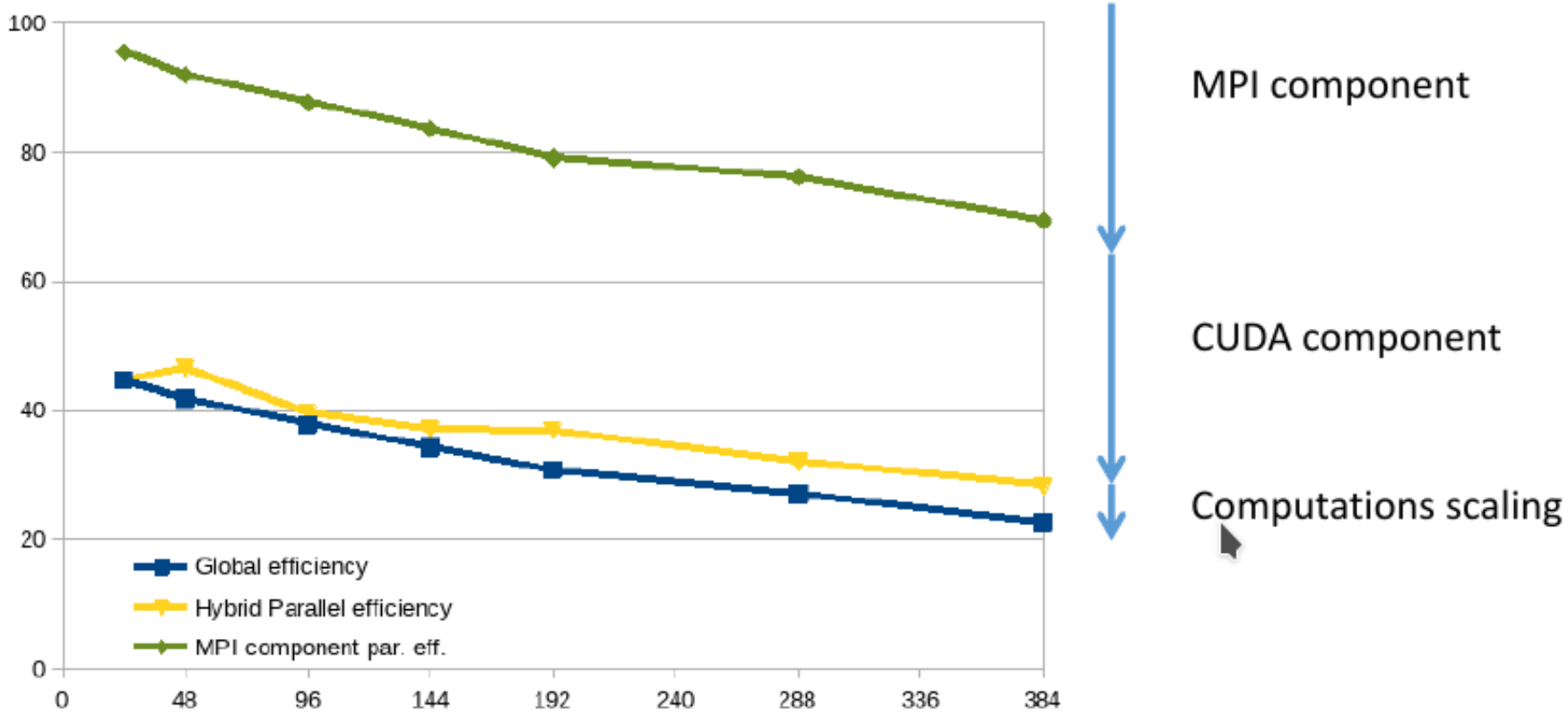
OpenMP parallel functions



OpenMP efficiencies [%]
- Parallel efficiency 93.51
- Load Balance 96.05
- Communication 97.39

→ Phase 2 only reports MPI imbalance as expected

Same approach applied to MPI+CUDA



- Bigger impact from CUDA component with a similar contribution in all the scales
- MPI contribution increases with the scale, but still lower than CUDA

How to calculate the metrics?

- We recommend the following Python tools to automatically calculate metrics from Extrae data
  - **NAG-PyPOP** for additive metrics (pip install [--user] NAG-PyPOP) (https://pypi.org/project/NAG-PyPOP)
  - **BSC's Basic Analysis** module for multiplicative metrics (https://tools.bsc.es/downloads)

- Scalasca + Cube have some POP metrics support (Score-P traces)
- Other tracing tools can be used as metrics can be calculated manually (see handouts for details)

- POP can do it for you!

Conclusions

- We presented two generic models to characterize the efficiency of hybrid codes by splitting the contribution of each programming model.
- Each model has its own strengths:
  - The additive approach is based on concepts specific to each programming model, making them easier to map to known problems.
  - Not focusing on the specifics of each parallel programming paradigm, the multiplicative approach allows us to use the same model with MPI+OpenMP, MPI+CUDA,…
- The two models are being used in the framework of the POP2 Center of Excellence (https://pop-coe.eu)

Performance Optimisation and Productivity

A Centre of Excellence in HPC

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