Extra-P:
Insightful Automatic Performance Modeling

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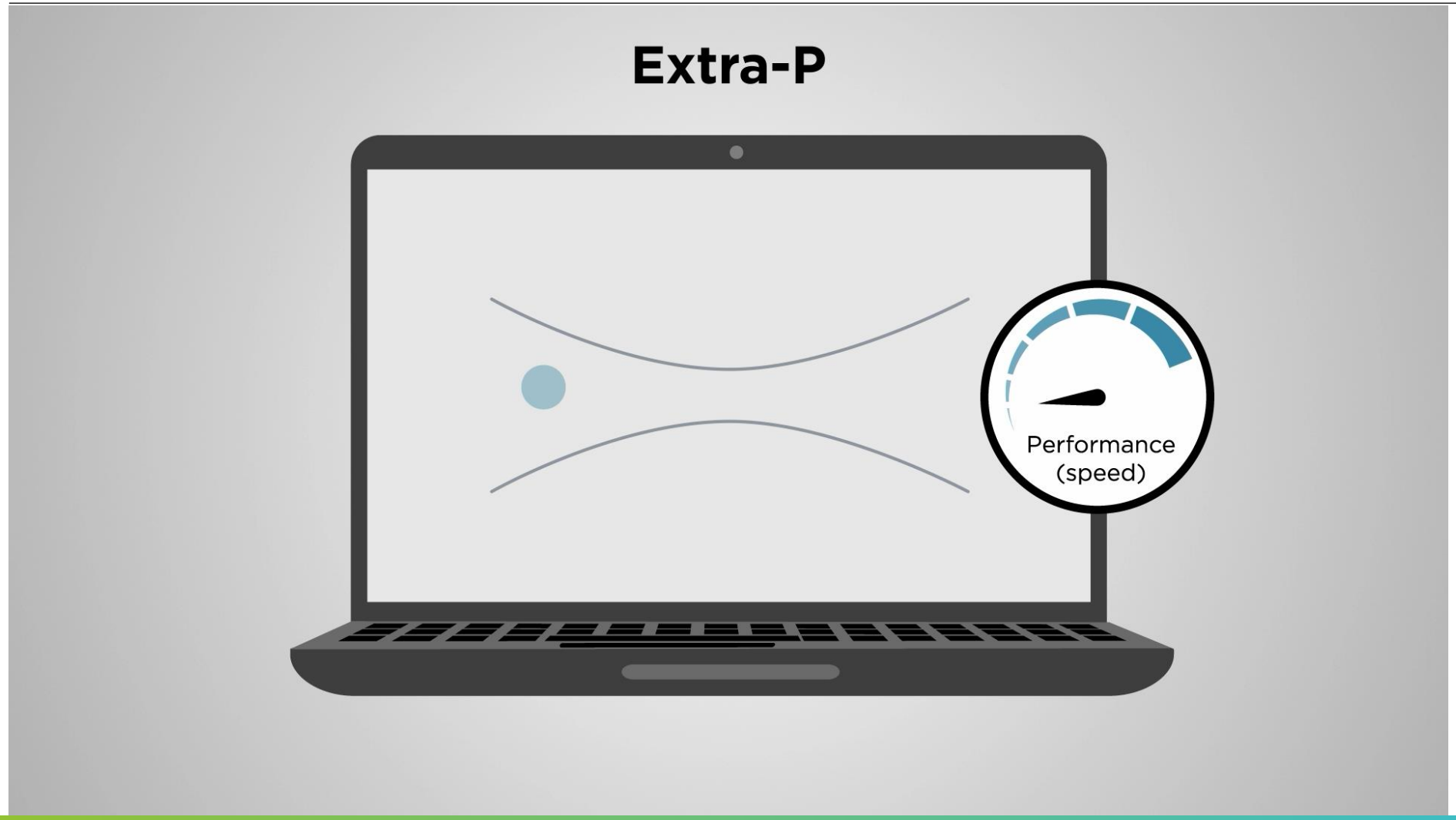
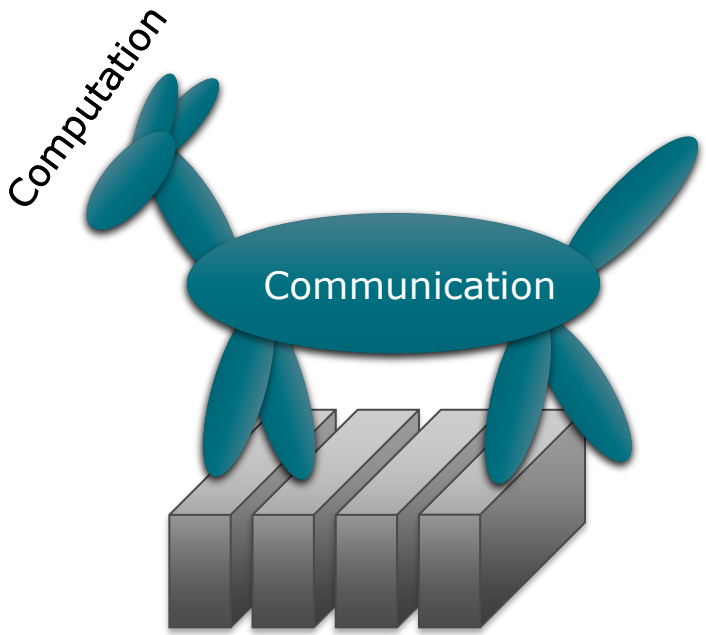
Introduction

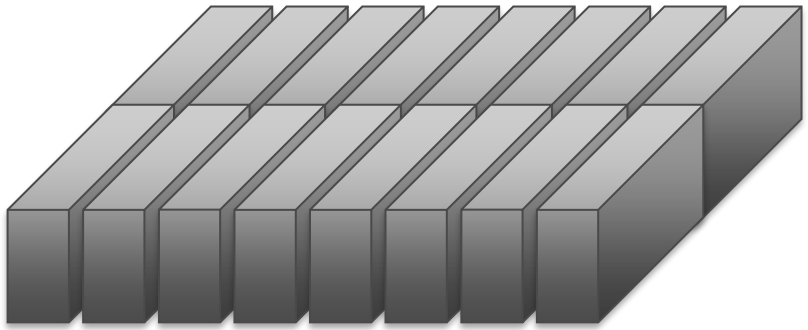


Watch Extra-P overview video

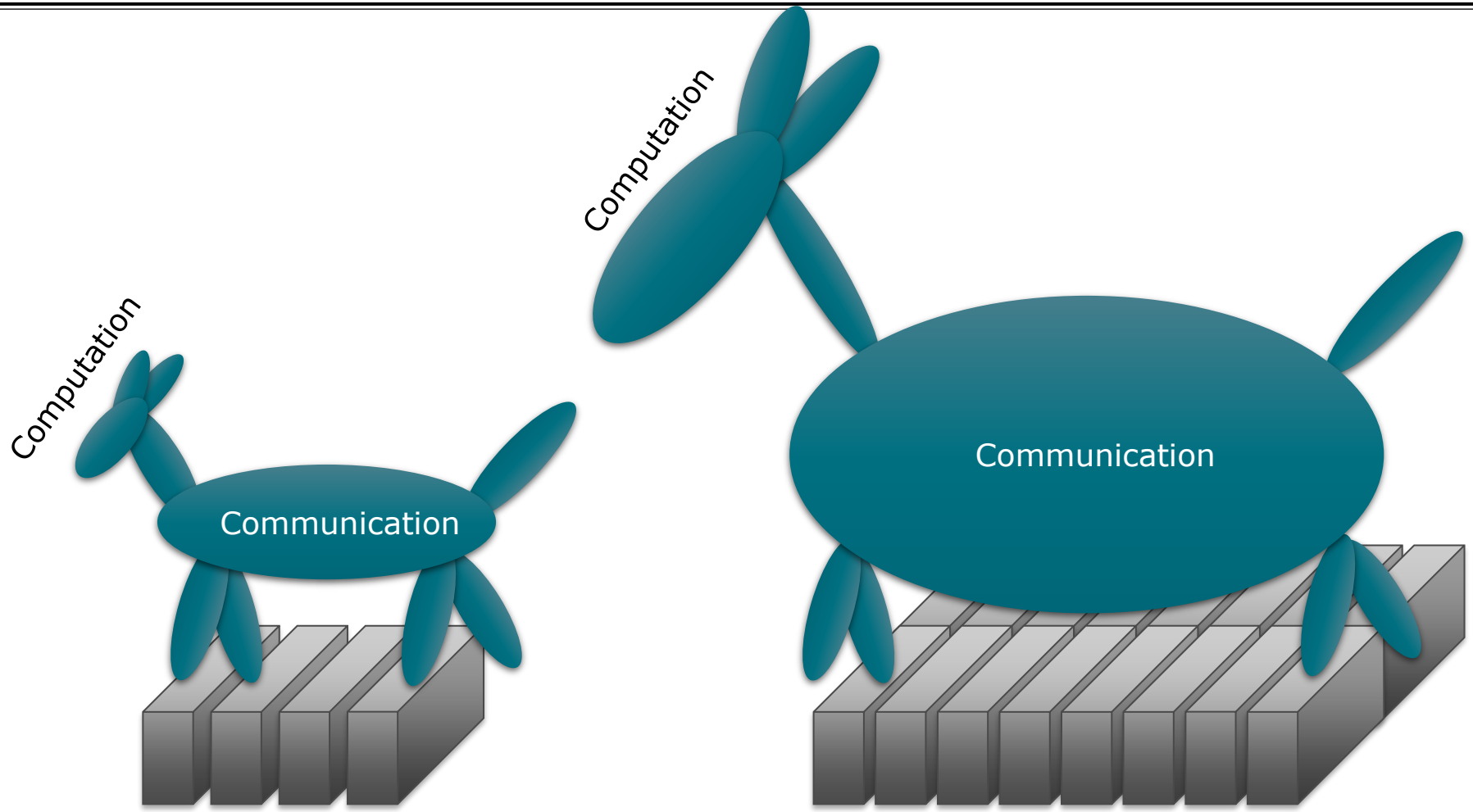
https://www.youtube.com/watch?v=Cv2YRCMWqBM

Motivation - latent scalability bugs



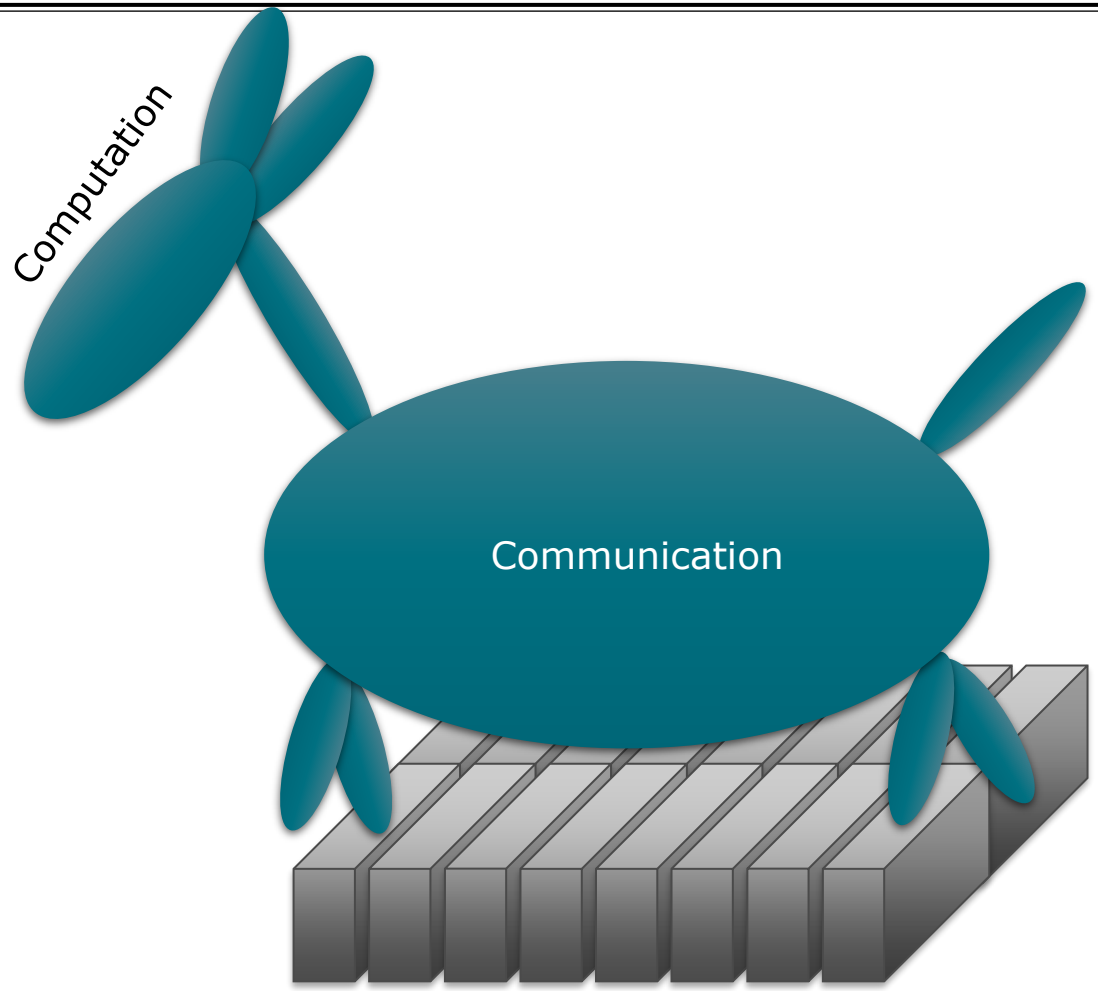


Scaling code to a bigger machine can unveil unpleasant surprises

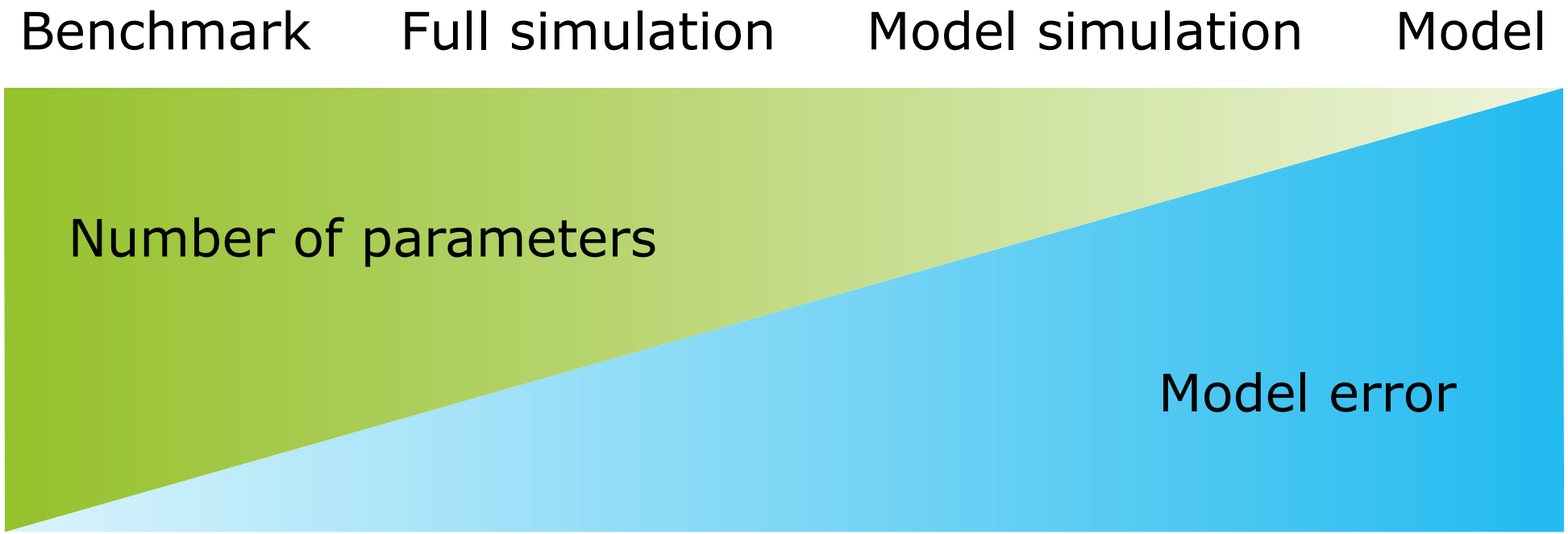


Scaling code to a bigger machine can unveil unpleasant surprises

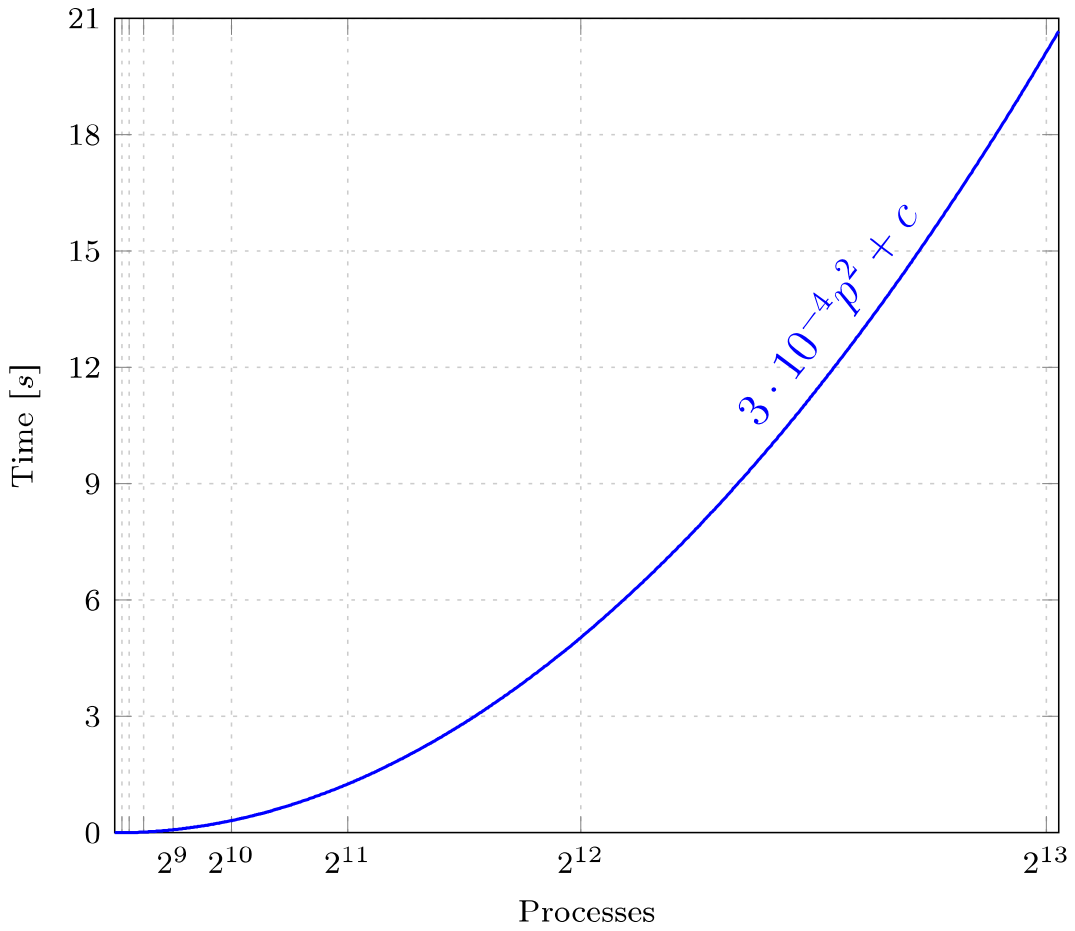
We need to find scaling issues before they occur



Spectrum of performance analysis methods



Scaling model



- Represents performance metric as a function of the number of processes
- Provides insight into the program behavior at scale

Analytical performance modeling

Identify kernels

- Parts of the program that dominate its performance at larger scales
- Identified via small-scale tests and intuition

Create models

- Laborious process
- Still confined to a small community of skilled experts

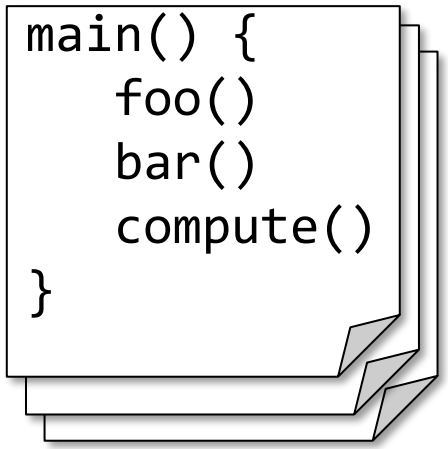
Disadvantages:

- Time consuming
- Danger of overlooking unscalable code

Hoisie et al.: *Performance and scalability analysis of teraflop-scale parallel architectures using multi-dimensional wavefront applications.* International Journal of High Performance Computing Applications,2000

Bauer et al.: *Analysis of the MILC Lattice QCD Application su3_rmd*. CCGrid, 2012

Automatic performance modeling



Input

Instrumentation

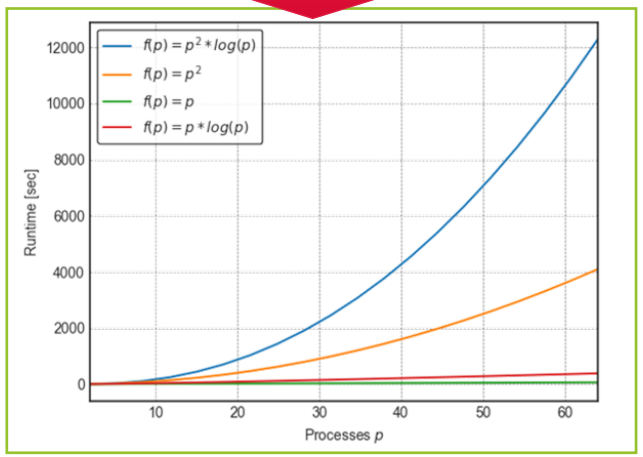
- All functions

Performance measurements

Extra-P

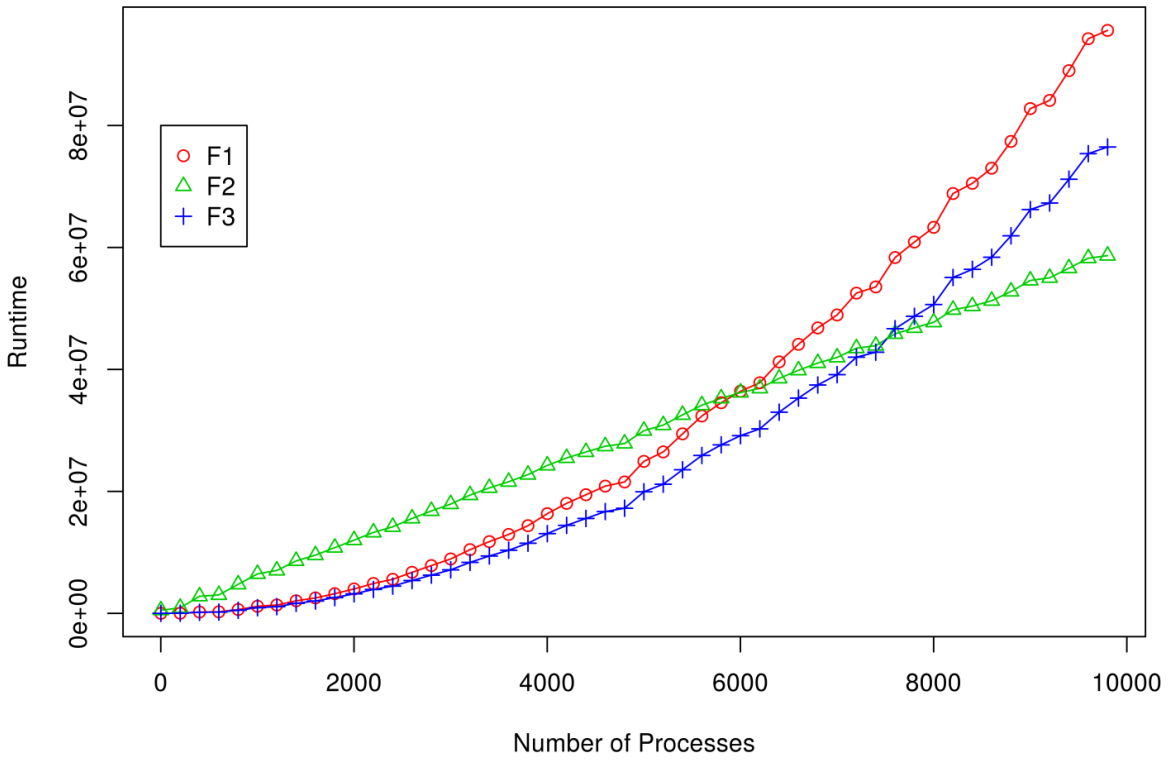
Output

Human-readable performance models of all functions (e.g., $t(p) = c_1 \cdot \log(p) + c_2$)

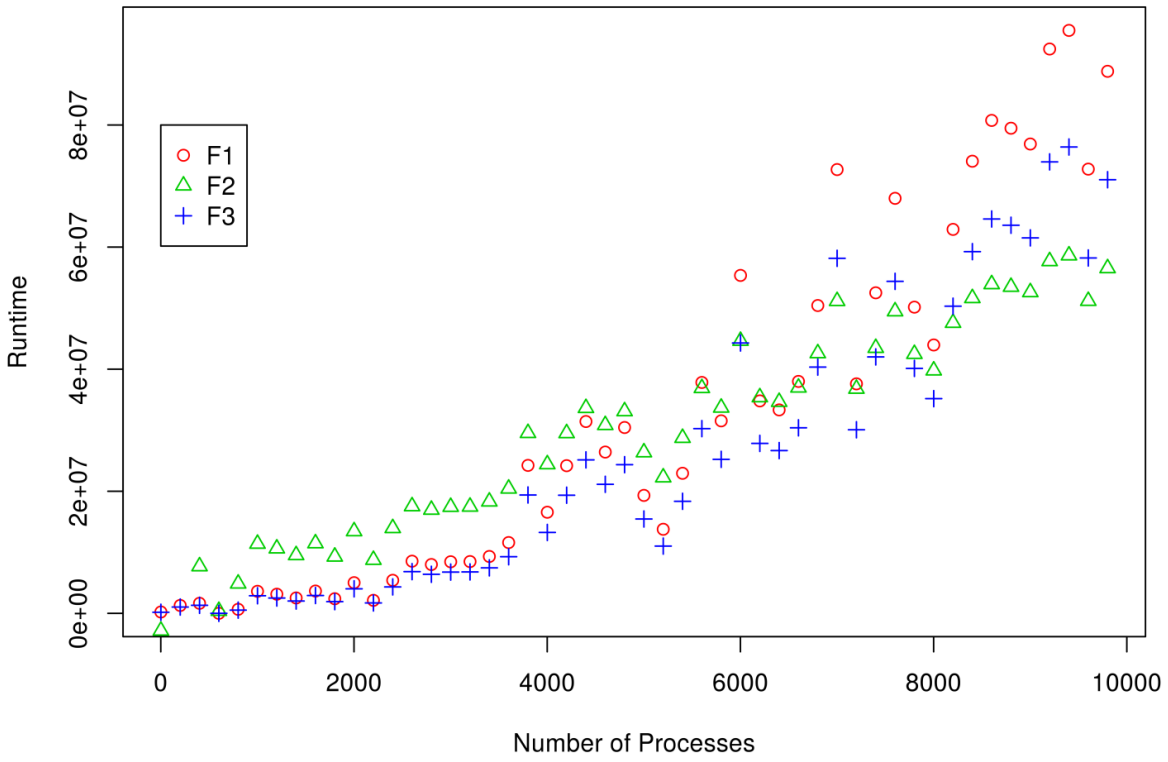


Primary focus on scaling trend

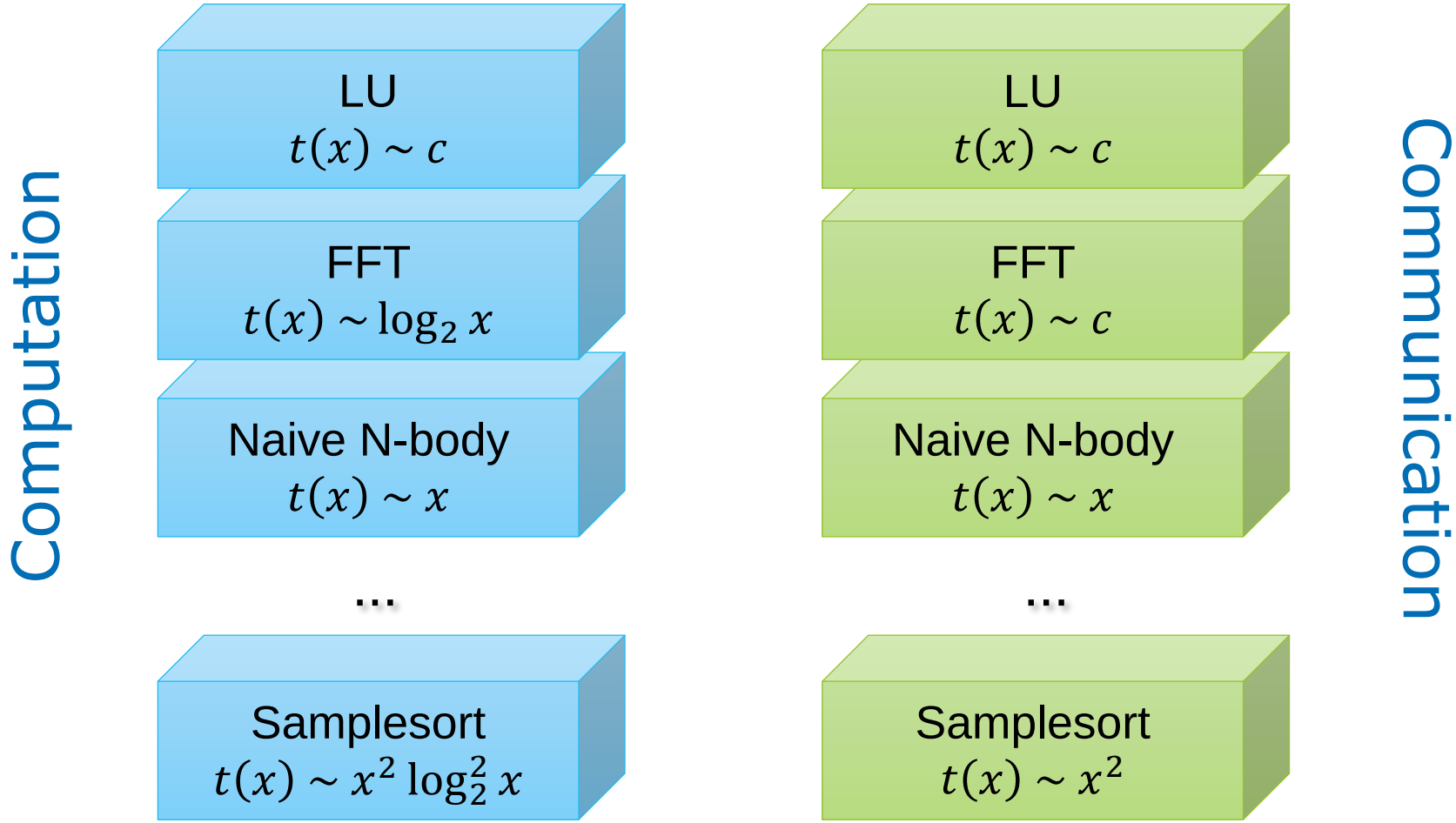
Common performance analysis chart in a paper



Production Reality



Model building blocks



Performance model normal form

$$f(x) = \sum_{k=1}^{n} c_k \cdot x^{i_k} \cdot log_2^{j_k}(x)$$

$$n \in \mathbb{N}$$
$$i_k \in I$$
$$j_k \in J$$
$$I, J \subset \mathbb{Q}$$

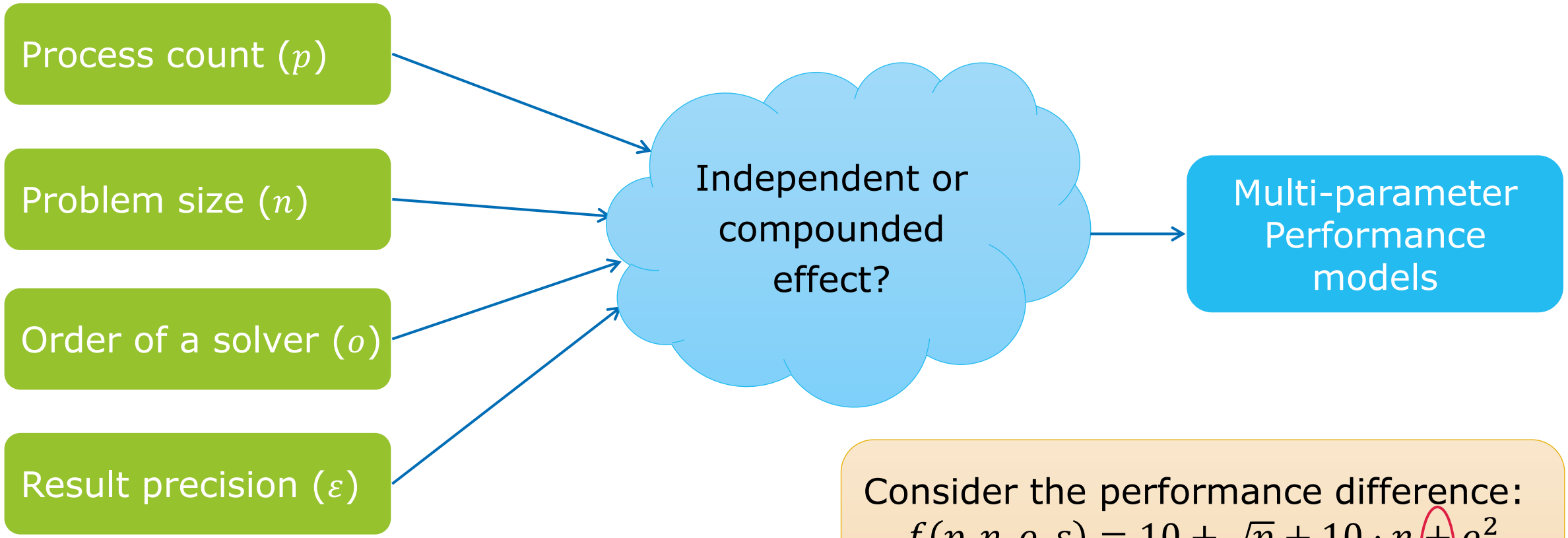
$$n = 1$$
$$I = \{0, 1, 2\}$$
$$J = \{0, 1\}$$

c_1 $\quad$ $c_1 \cdot \log x$

$c_1 \cdot x$ $\quad$ $c_1 \cdot x \cdot \log x$

$c_1 \cdot x^2$ $\quad$ $c_1 \cdot x^2 \cdot \log x$

Fast multi-parameter performance modeling



Consider the performance difference:

$$f(p,n,o,\varepsilon) = 10 + \sqrt{p} + 10 \cdot n + o^2$$

$$f(p,n,o,\varepsilon) = 10 + \sqrt{p} + 10 \cdot n \cdot o^2$$

Fast multi-parameter performance modeling

- Expanded performance model normal form

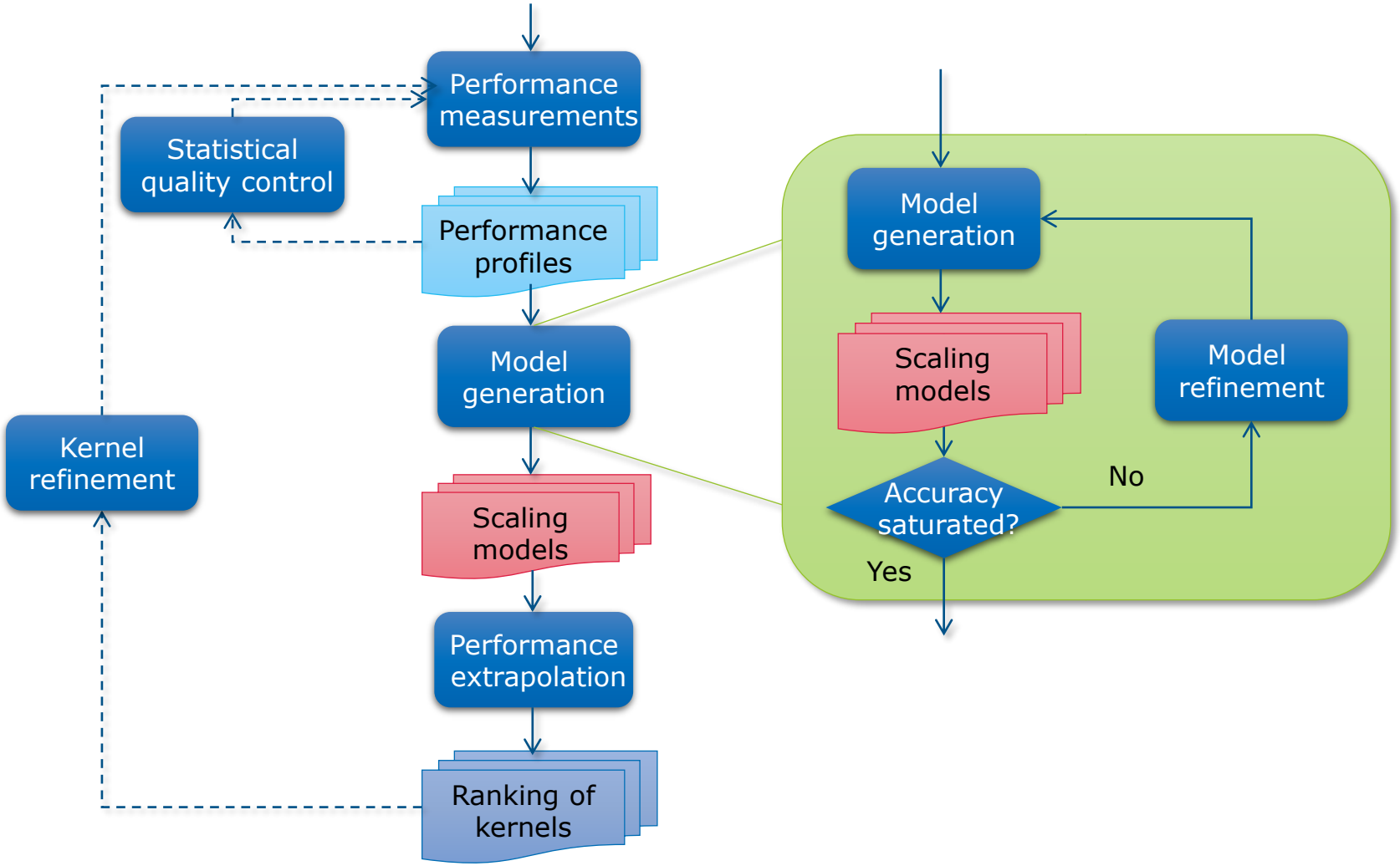
$$f(x_1, \ldots, x_m) = \sum_{k=1}^{n} c_k \prod_{l=1}^{m} x_l^{i_{kl}} \cdot log_2^{j_{kl}}(x_l)$$

$$m, n \in \mathbb{N}$$
$$i_k \in I$$
$$j_k \in J$$
$$I, J \subset \mathbb{Q}$$

Model candidates

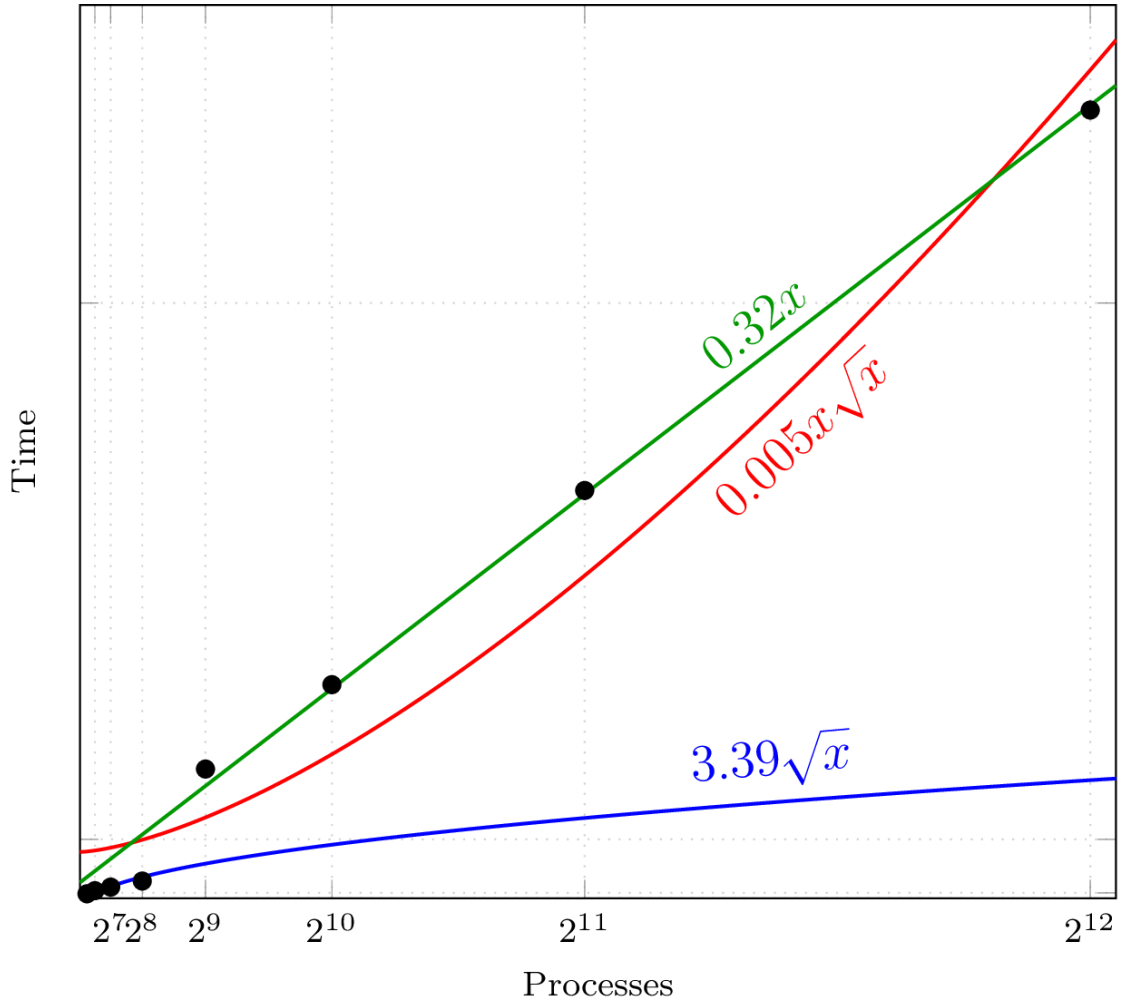
- Constant c_1
- Single parameter $c_1 + c_2 \cdot x_1$
- Multiple parameters …
  - Additive $c_1 + c_2 \cdot x_1 + c_3 \cdot x_2$
  - Multiplicative $c_1 + c_2 \cdot x_1 \cdot x_2$
  - Complex $c_1 + c_2 \cdot x_1 \cdot x_2 + c_3 \cdot \log x_2 \cdot x_2^3$

Workflow


Performance measurements
Statistical quality control
Performance profiles
Model generation
Kernel refinement
Scaling models
Performance extrapolation
Ranking of kernels
Model generation
Scaling models
Model refinement
Accuracy saturated?
No
Yes

Assumptions & limitations

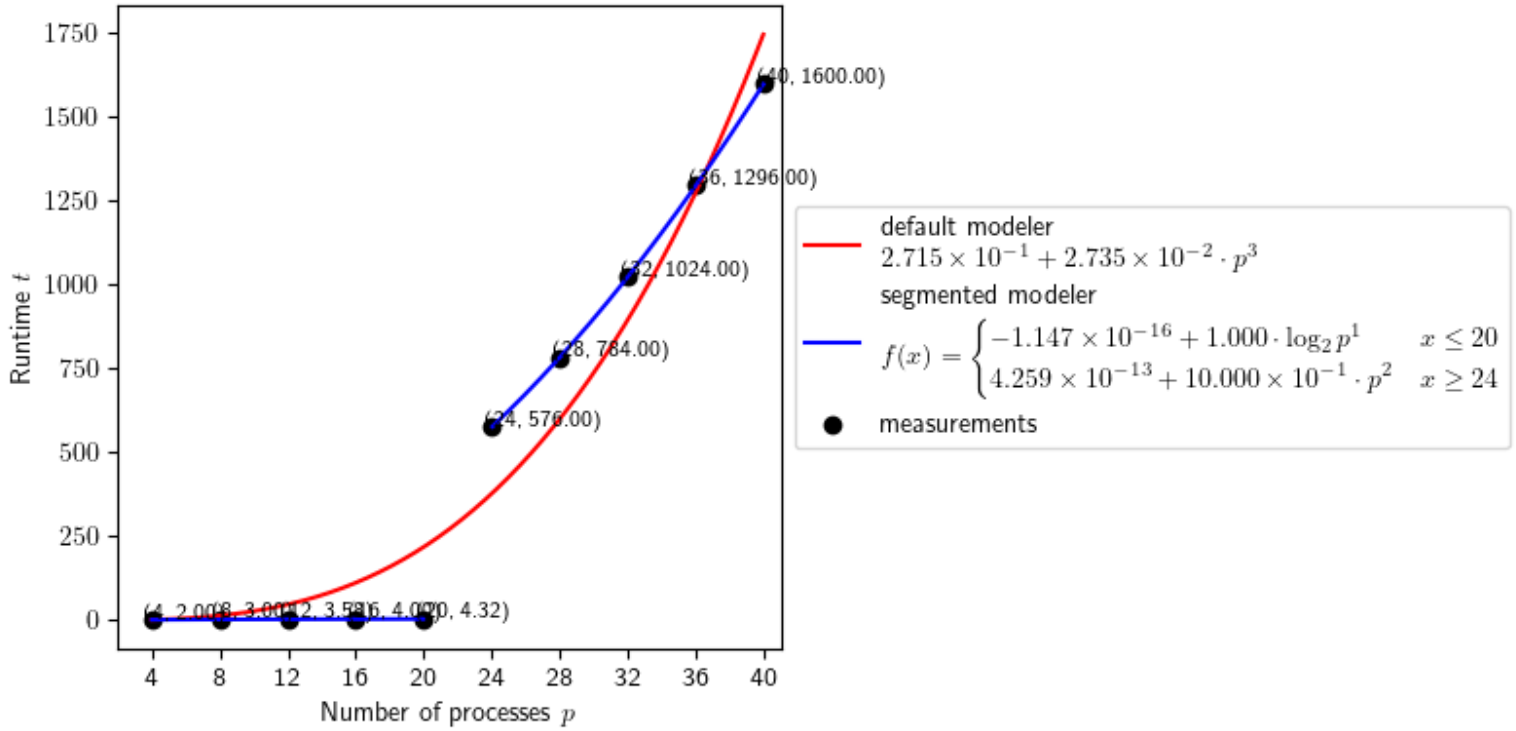
- Scaling behavior expressible with performance model normal form
- Only one scaling behavior for all the measurements; no jumps
- Some MPI collective operations switch their algorithm
  - results in bad models
- Example: red model tries to model measurements of different algorithms
  - First 4 points – one function
  - Last 4 points – another function (linear)
  - Adj. R2 = 0.95085 (!)



Segmented models

Beta

- We can detect and model segmented behavior
- When enough measurement points are present
- Segmented modeler must be manually selected
- Limited to two segments

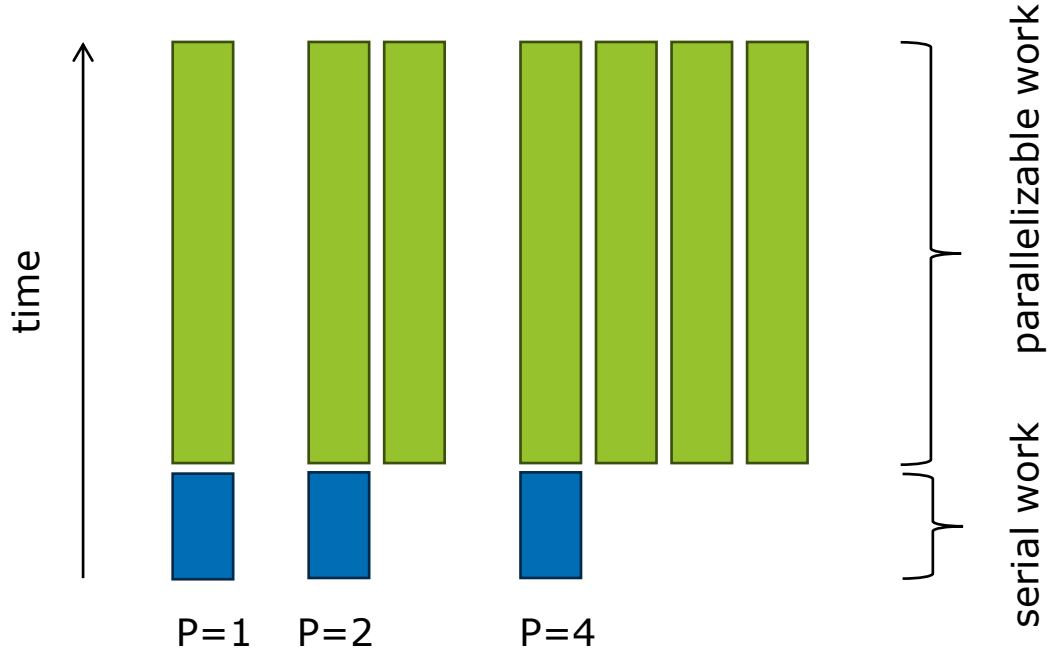


Scaling analysis: number of processes is increased

Preferred by Extra-P

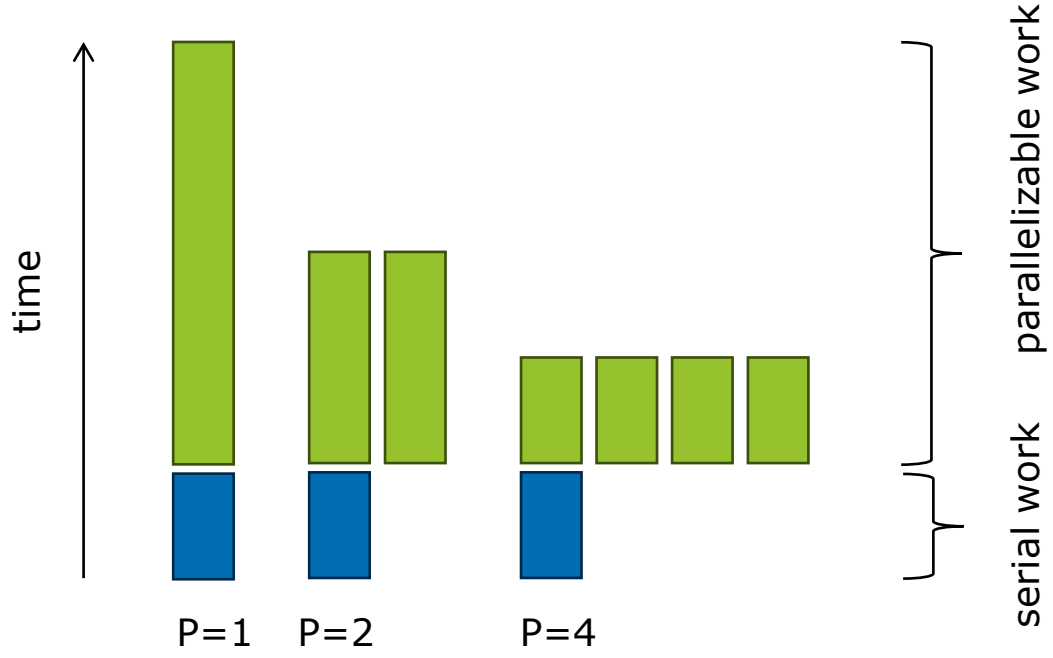
Weak scaling

- The problem size is increased alongside
- Law of Gustafson



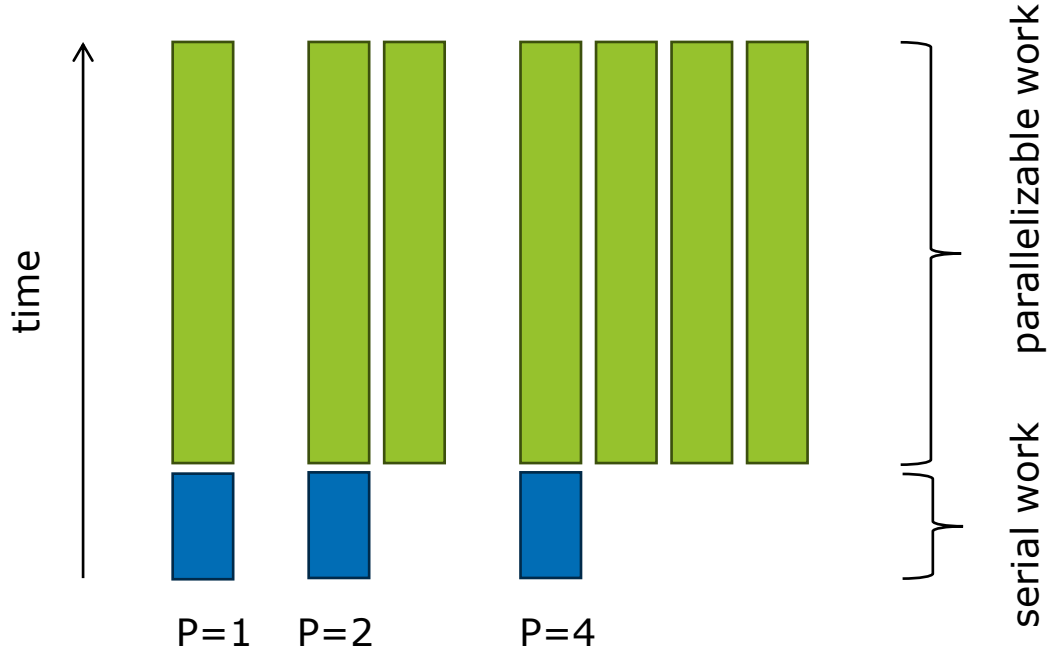
Strong scaling

- The problem size remains constant
- Amdahl's law

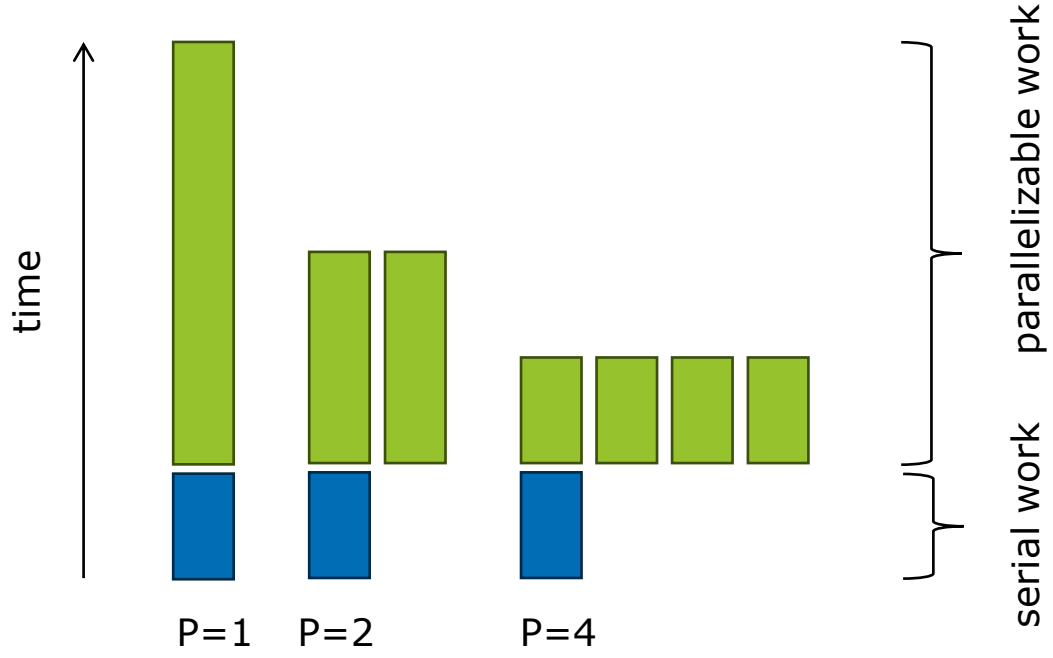


Scaling analysis with Extra-P

Weak scaling



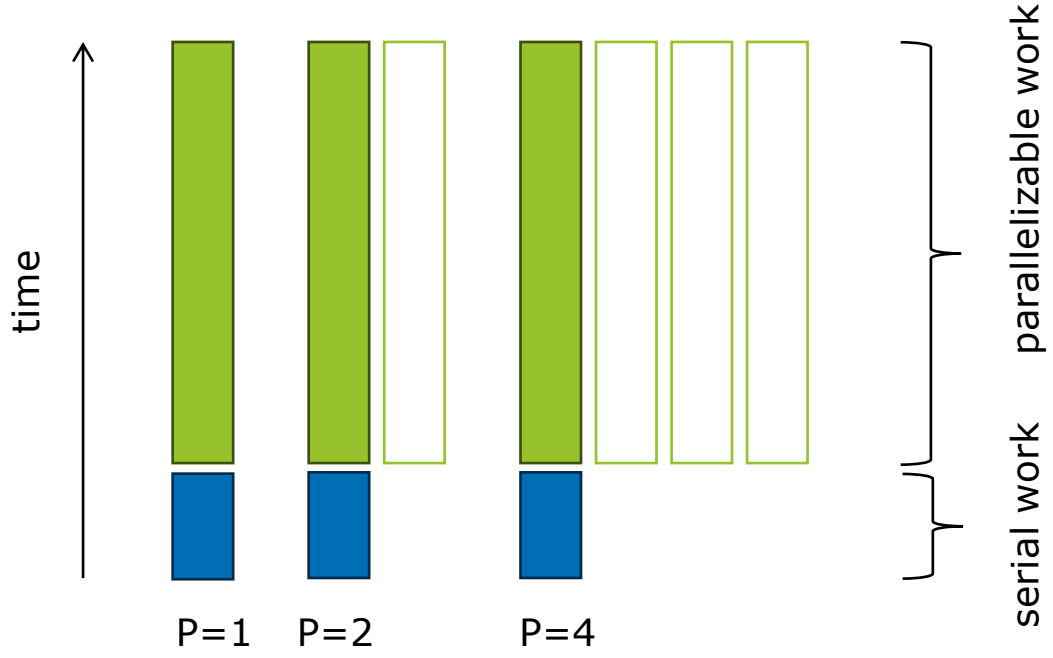
Strong scaling



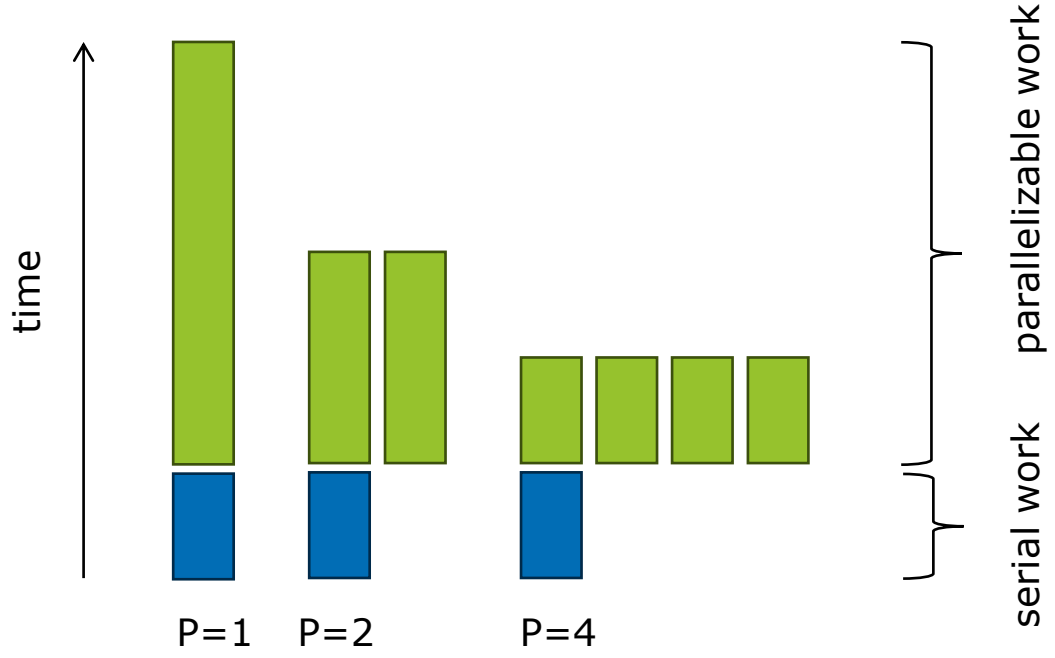
Scaling analysis with Extra-P

Weak scaling

- Extra-P models the runtime of one process



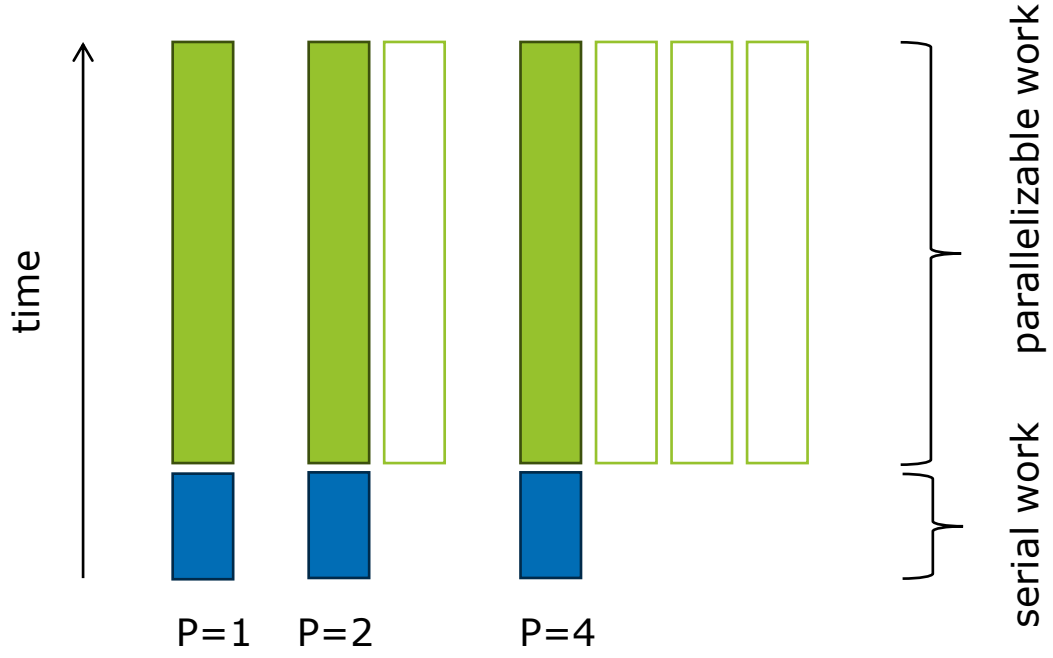
Strong scaling



Scaling analysis with Extra-P

Weak scaling

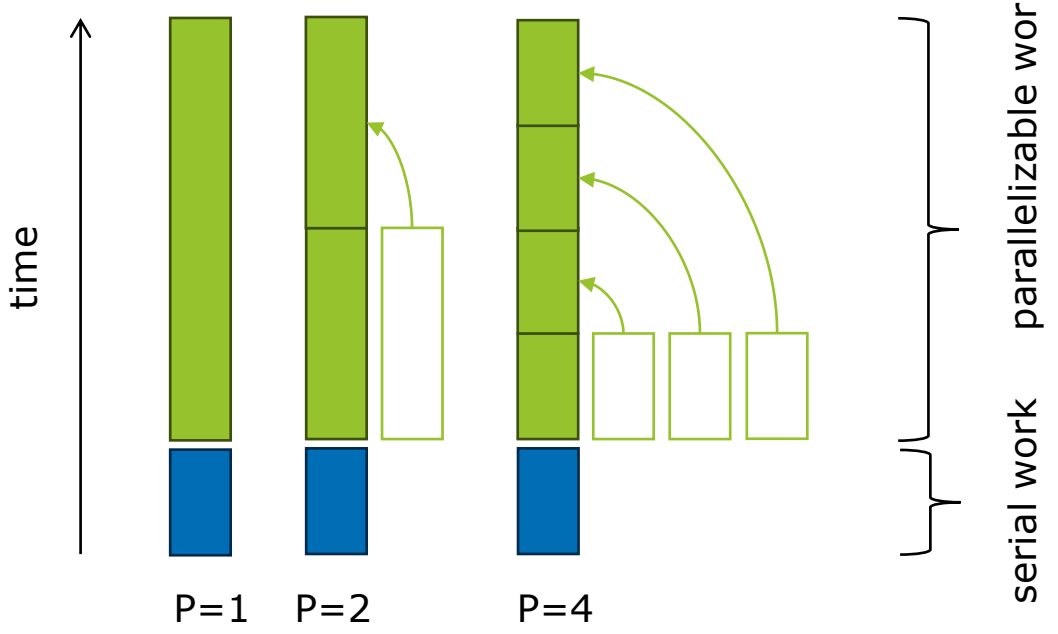
- Extra-P models the runtime of one process



Strong scaling

- Extra-P models the resource consumption
  - Runtime of all processes combined
  - Equivalent to the number of core-hours
  - Automatic detection and conversion

Beta



Performance measurements

Different ways of collecting measurements

- Score-P (http://www.vi-hps.org/projects/score-p/)
- Other profiling tools, e.g. HPCToolkit
- Manual ad-hoc measurements

Performance measurements (2)

- At least 5 different measurements recommended

Performance measurements (profiles)

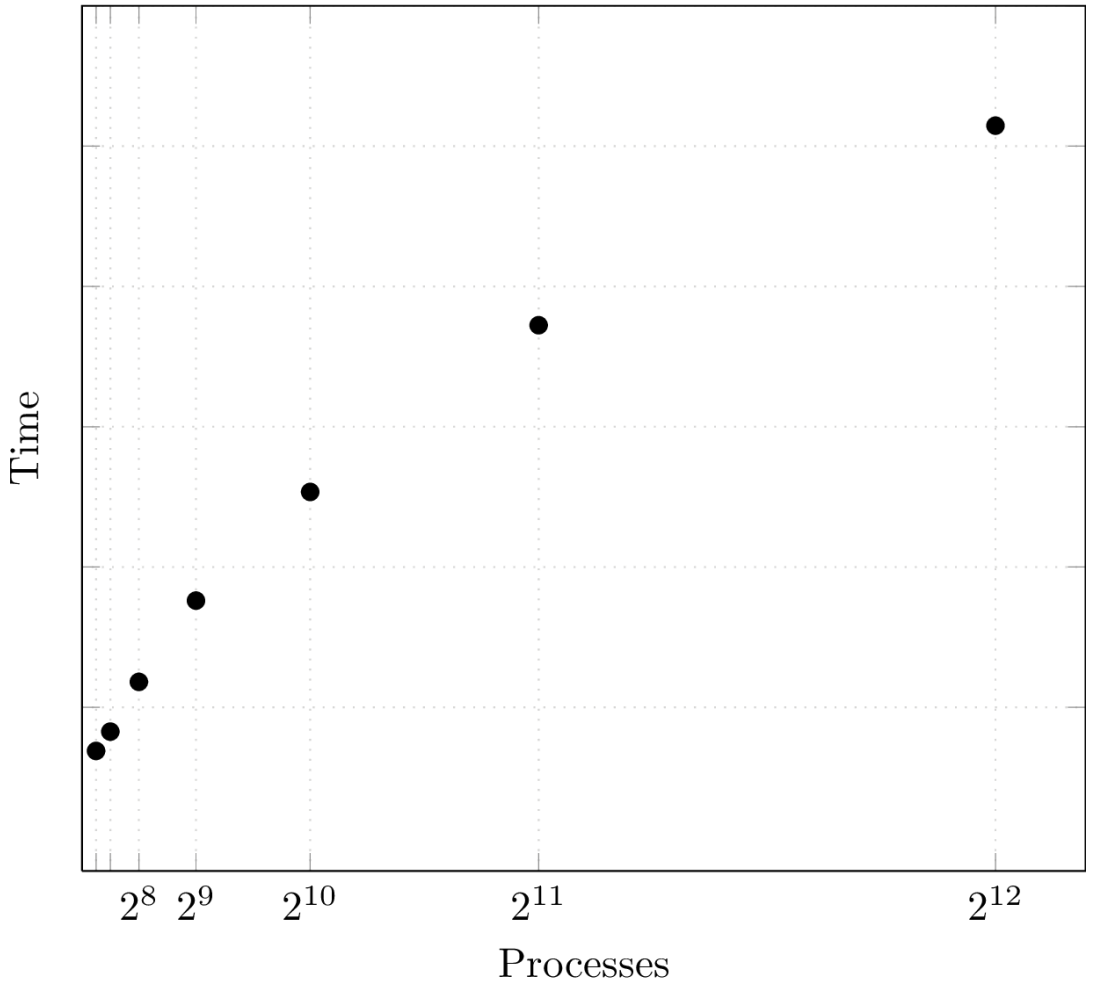
$p_1 = 256$

$p_2 = 512$

$p_3 = 1024$

$p_4 = 2048$

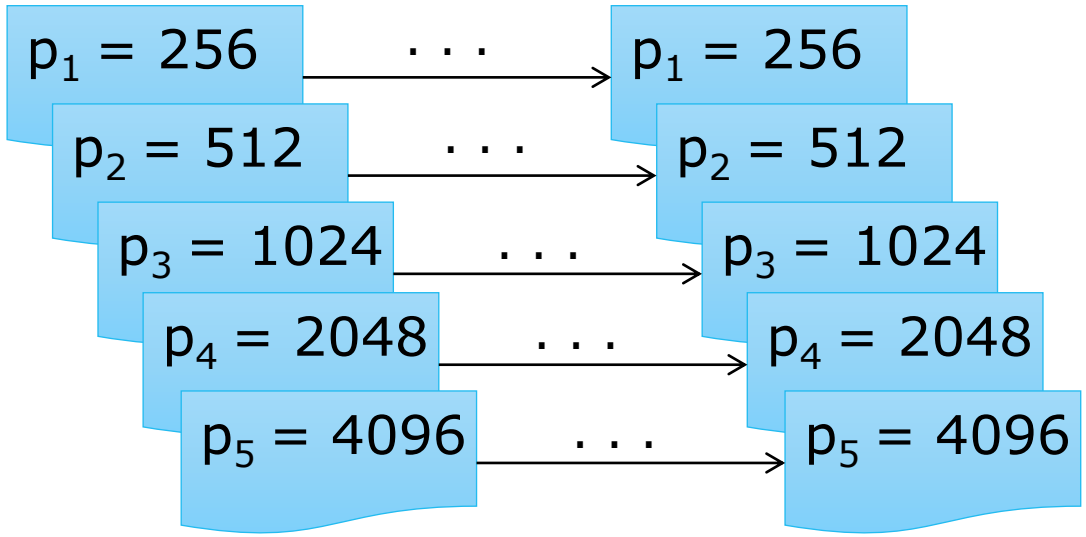
$p_5 = 4096$

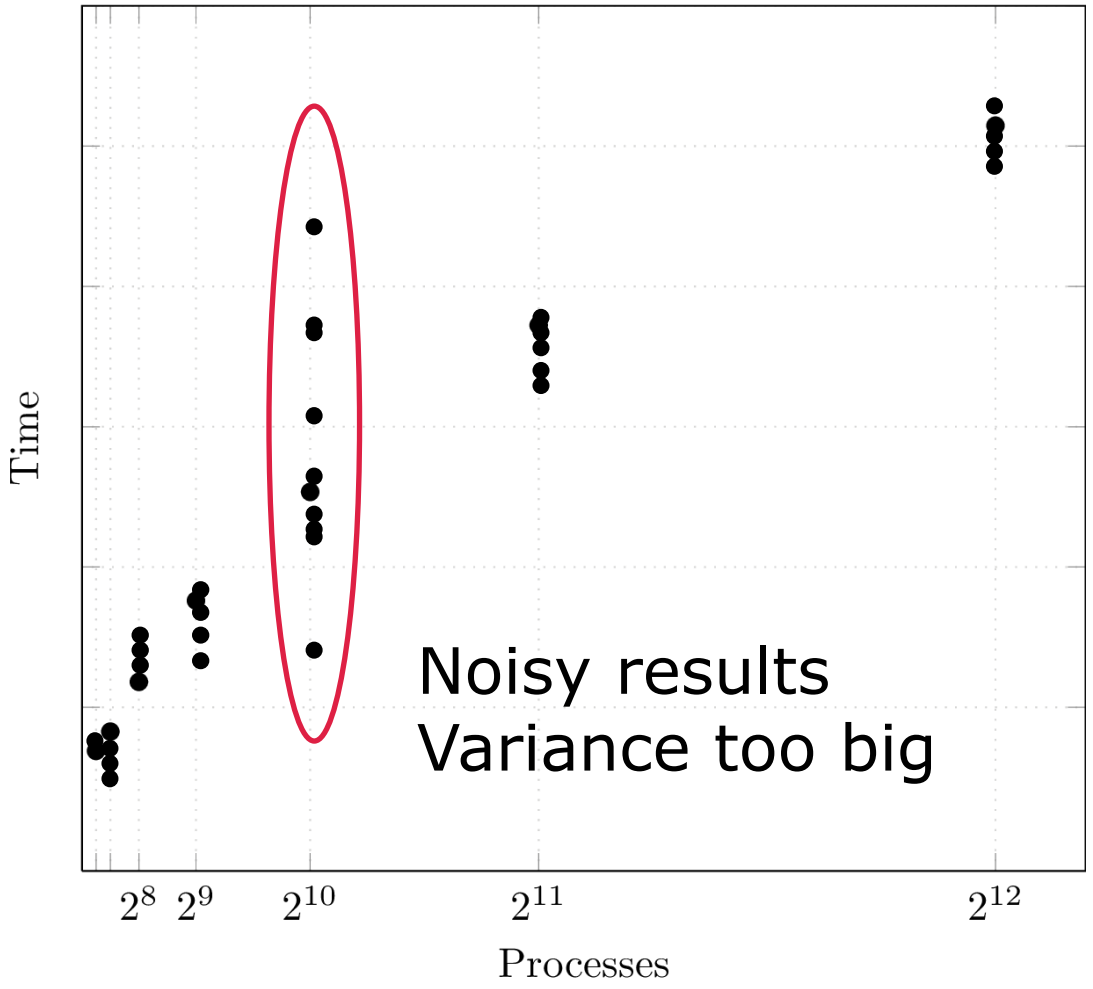


Performance measurements (3)

- At least 5 different measurements recommended
- Each measurement repeated multiple times

Performance measurements (profiles)





Adjusted R^2

- R^2 represents how well the determined function fits the M available measurements

- Adjusted R^2 adjusts for N, the number of terms used
  - Adj. R^2 decreases → more useless variables
  - Adj. R^2 increases → more useful variables

- Rule of thumb: adj. $R^2 > 0.95$

$$R^2 = 1 - \frac{\text{residualSumSquares}}{\text{totalSumSquares}}$$

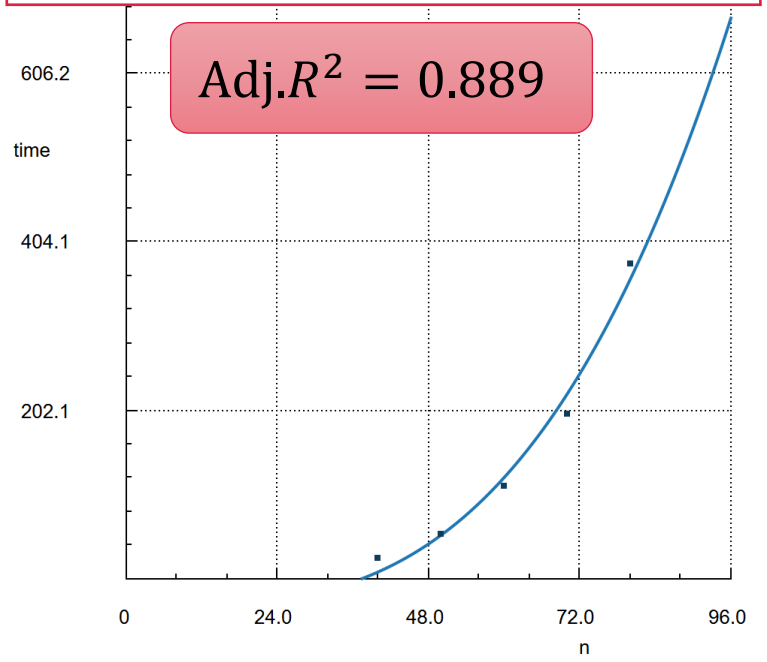
$$\overline{R^2} = 1 - (1 - R^2) \cdot \frac{M - 1}{M - N - 2}$$

Quadratic and cubic problems

- The whole problem size should be used as parameter
  - Not just the edge length

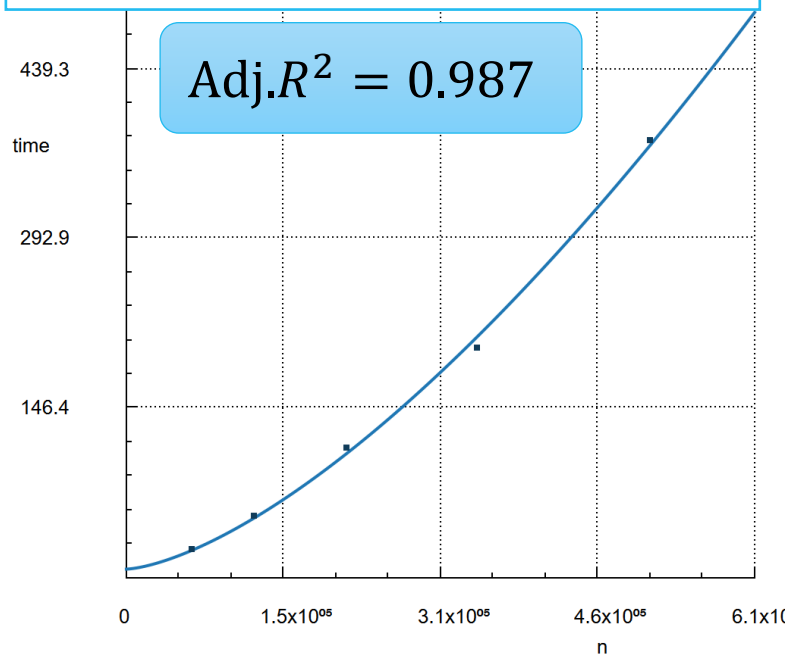
Edge length: n

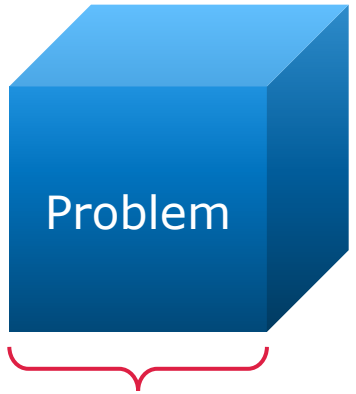
$-32.98 + 0.000121 * n^3 * \log2(n)$



Volume: n

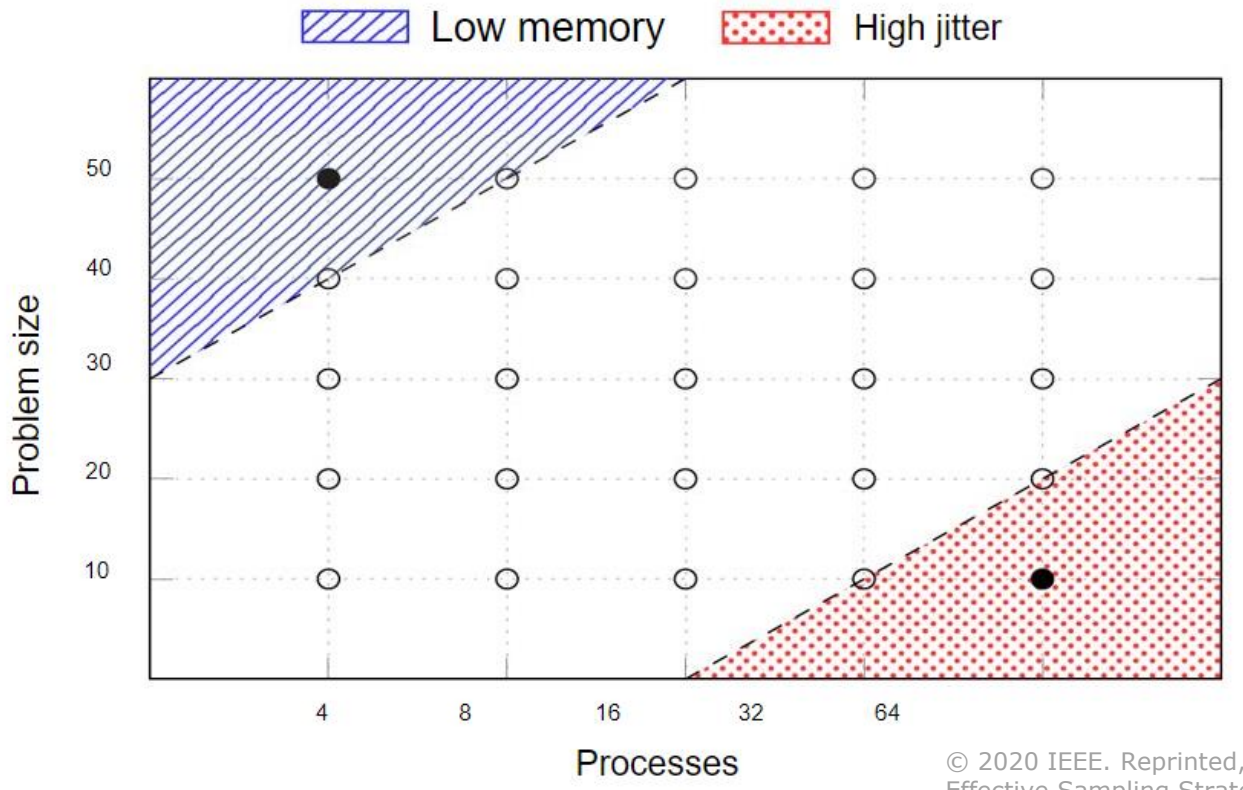
$7.53 + 9.98 \cdot 10^{-7} * n^{1.5}$





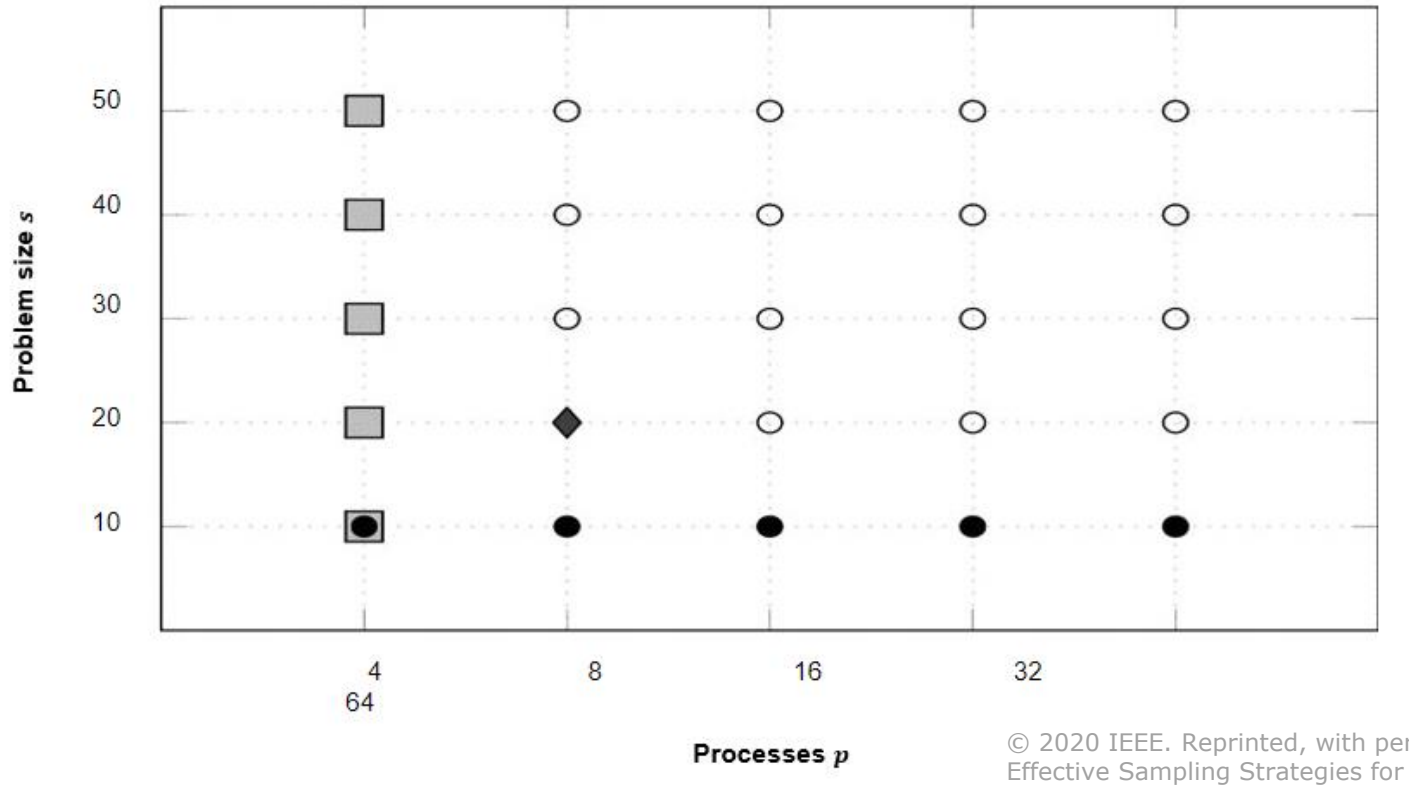
Sparse modeling

- Experiments can be expensive
- So far we needed 5×5^m experiments, m=number of parameters



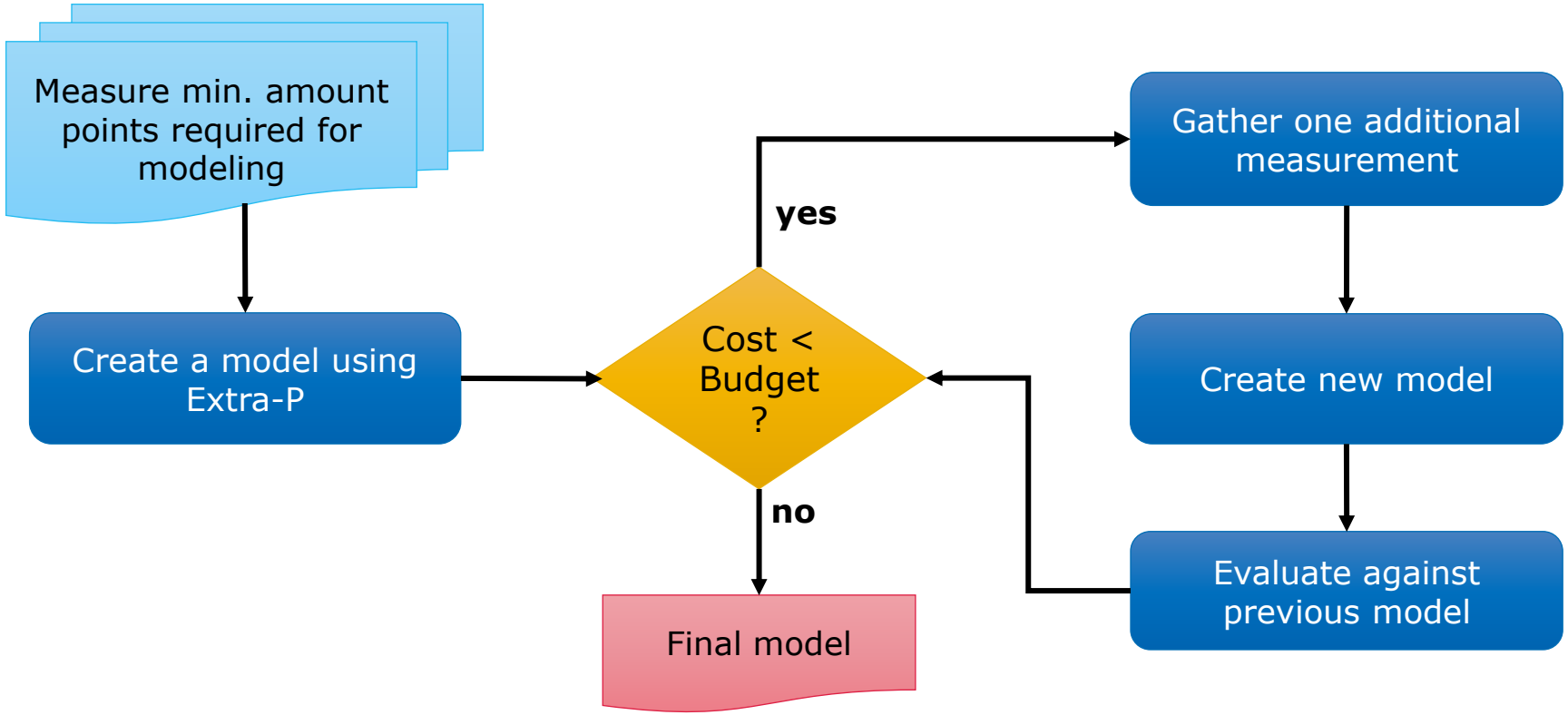
Sparse modeling

- Using our new sparse modeling approach we can model with less points!
- We only need $5 \times 5 \cdot m$ experiments, m=number of parameters



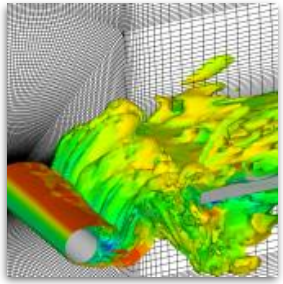
Sparse modeling

- Recommended experiment configuration strategy using our heuristic guideline



Sparse modeling

- Using sparse modeling we can reduce the average modeling cost by ~85% (on synthetic data)
- We can retain ~92% of the model accuracy (on synthetic data)
- Allows a more flexible experiment design



FASTEST
- 70% decrease in cost
- ~2% prediction error

Image by Institute for Numerical Methods in Mechanical Engineering, TU Darmstadt

Kripke
- 99% decrease in cost
- ~39% prediction error

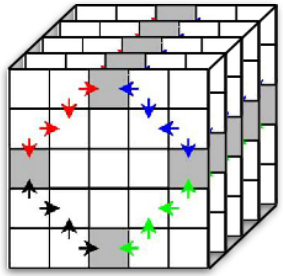


Image by Lawrence Livermore National Laboratory (CC BY-NC-SA 4.0)

Relearn
- 85% decrease in cost
- ~11% prediction error

Using Extra-P

Installing Extra-P

- Easy to install via pip
- Just run: `python -m pip install extrap --upgrade --pre`
  - The `--upgrade` forces the installation of a new version
- All dependencies (packages) will be installed automatically

To get the beta version

Extra-P in the tuning workshop

- Available at: https://github.com/extra-p/extrap

- When installed on the system simply run:
  - `extrap` – for the command line version
  - `extrap-gui` – for the graphical user interface version
- The GUI version is not intended to be used on the cluster

Automatic performance modeling with Extra-P

```
Myapp.cpp
main() {
    foo()
    bar()
    compute()
}
```

Instrumentation & Measurement

Score-P

Performance measurements (profiles)

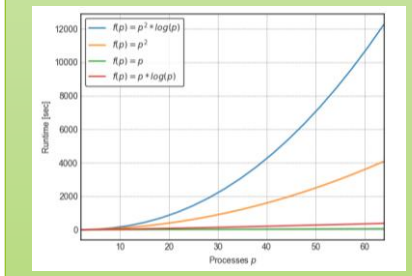
- Myapp.weak.p128.r1/profile.cubex
- Myapp.weak.p256.r1/profile.cubex
- Myapp.weak.p512.r1/profile.cubex
- Myapp.weak.p1024.r1/profile.cubex
- Myapp.weak.p2048.r1/profile.cubex

Input

Extra-P

Output

Results (visual)



Results (textual)

```
Region 1: main
Model: (3) + (3.14 * x^( 2 ))
...
```

Modeling sets of CUBE experiments

Extra-P Cube input description

Modeling tool expects CUBE files in the following format:

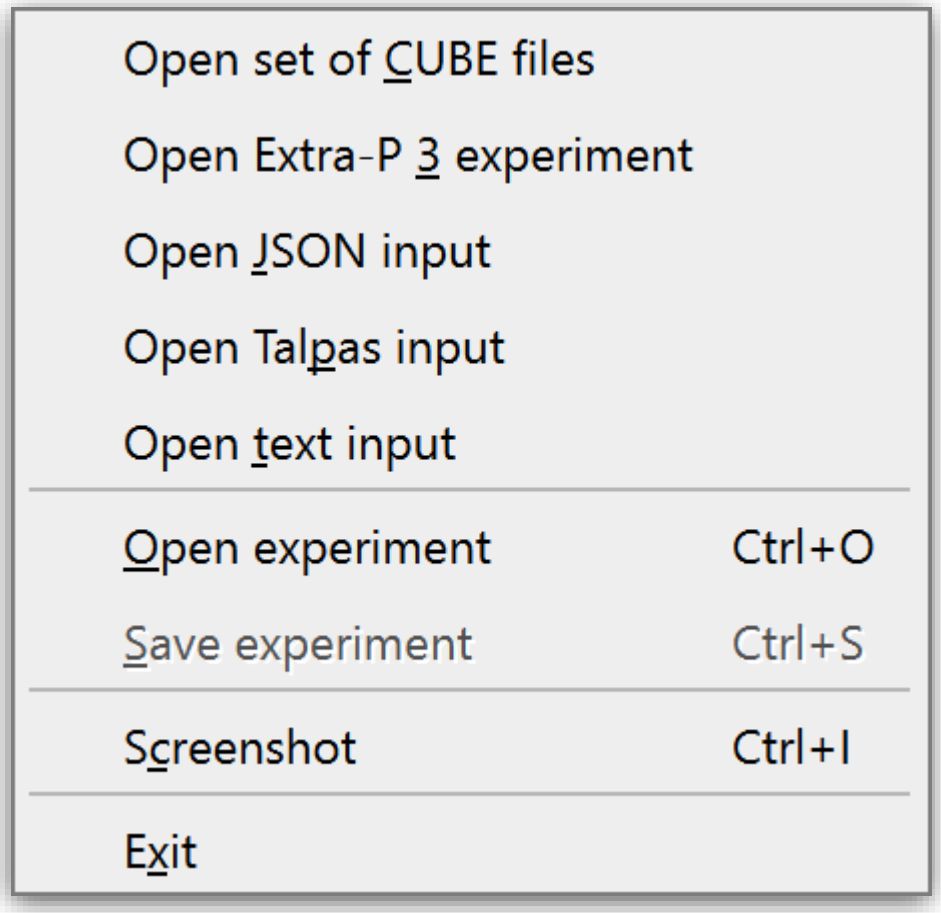
- <DIR>/<PREFIX>.<PARAMETERS>.r<REPETITION>/<FILENAME>.cubex
  - DIR, PREFIX, FILENAME – are just names, no meaning for Extra-P
  - REPETITION – number of the repetition of the experiments with same parameter values

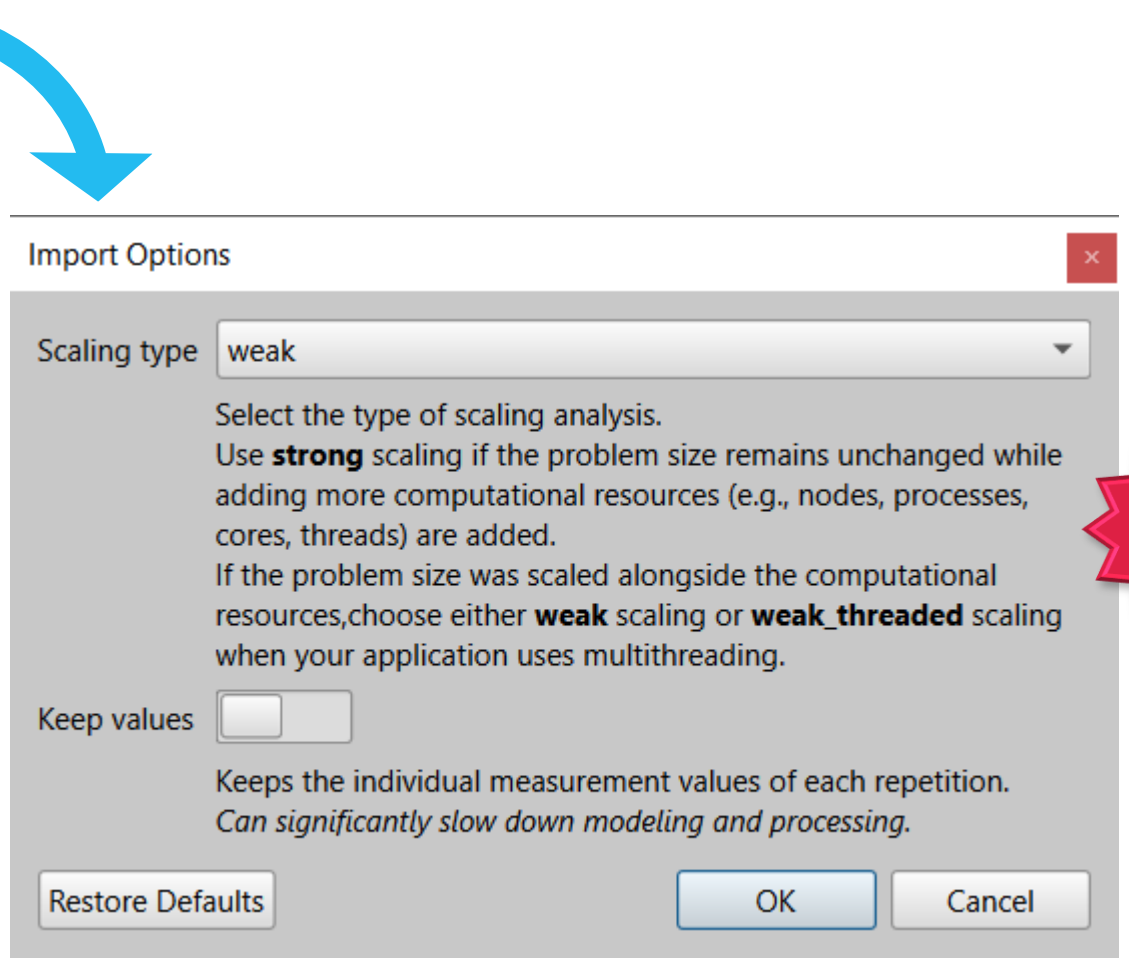
- <PARAMETERS>:=<PARAM1><VALUE1>.⋯.<PARAMn><VALUEn>
  - List of parameter-value-pairs separated by "."
  - PARAM – varied parameter e.g. number of processes
  - VALUE – value of the varied parameter

Extra-P Cube input description – example

- app.processes2.size8000.r1
- app.processes2.size8000.r2
- app.processes2.size8000.r3
- app.processes2.size8000.r4
- app.processes2.size16000.r1
- …
- app.processes2.size40000.r1
- app.processes4.size8000.r1
- …
- app.processes4.size40000.r4
- app.processes8.size8000.r1
- …
- app.processes8.size40000.r4
- app.processes16.size8000.r1
- …
- app.processes16.size40000.r4
- app.processes32.size8000.r1
- …
- app.processes32.size40000.r4

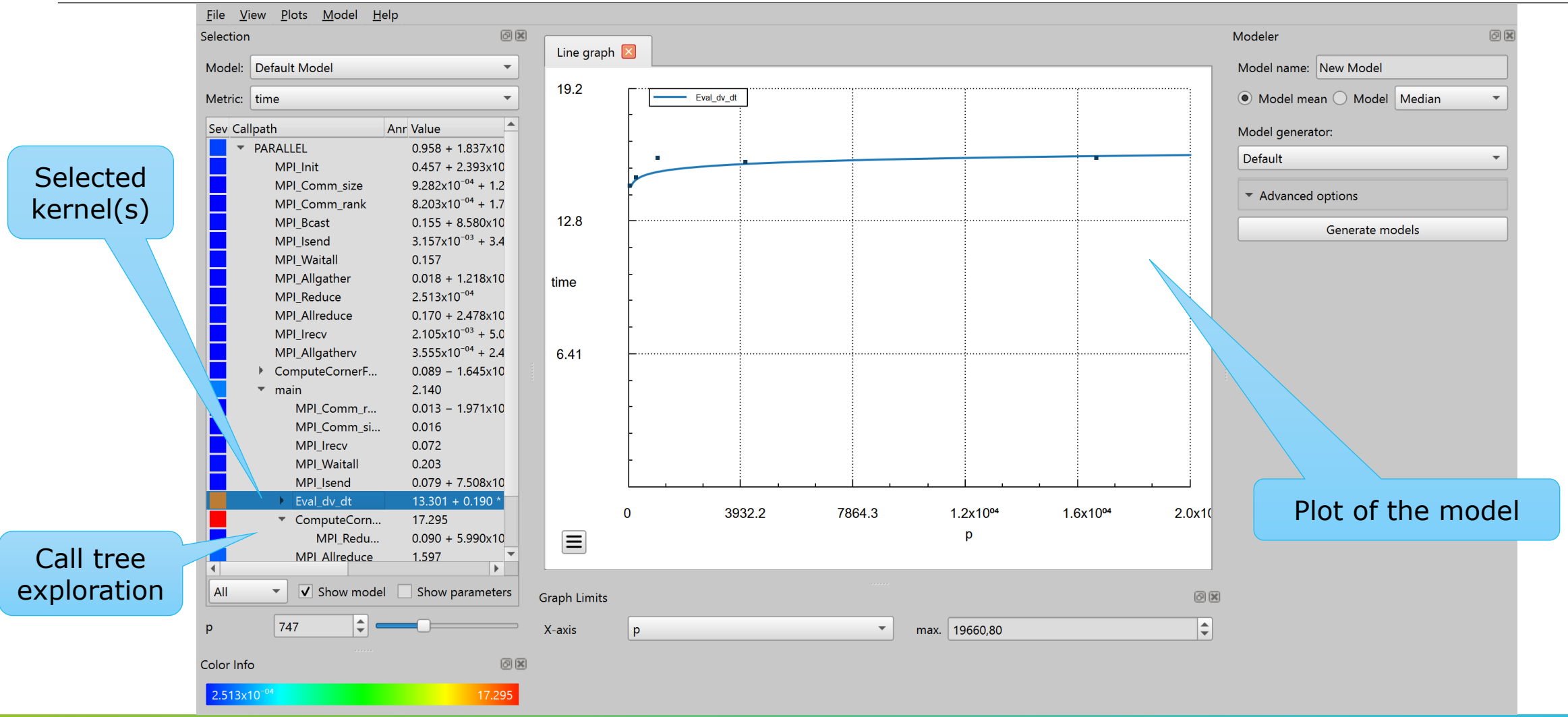
Extra-P Cube input





Visualization with Extra-P

Extra-P user interface



Extra-P call tree view

Metric selection

Model selection

Call tree exploration

Model

Quality of fit metrics: Residual sum of squares and Adjusted R^2

Impact of each kernel on the metric at the selected process count compared to the other kernels

Asymptotic behavior

Model: Default Model

Metric: time

Sev	Call	Anr	Value	RSS	Adj. R^2	SMAPE	RE
	PARALLEL		$0.958 + 1.837\text{x}10^{-05} * p * \log_2(p)$	0.092	0.990	2.903	0.029
	MPI_Init		$0.457 + 2.393\text{x}10^{-10} * p^{9/4}$	4.871x10...	0.998	0.829	$8.259\text{x}10^{-03}$
	MPI_Comm_size		$9.282\text{x}10^{-04} + 1.232\text{x}10^{-09} * p * \log_2(p)$	8.406x10...	0.981	1.096	0.011
	MPI_Comm_rank		$8.203\text{x}10^{-04} + 1.796\text{x}10^{-10} * p * \log_2(p)$	1.241x10...	0.987	0.155	$1.552\text{x}10^{-03}$
	MPI_Bcast		$0.155 + 8.580\text{x}10^{-11} * p^{7/3}$	6.011x10...	0.997	3.815	0.038
	MPI_Isend		$3.157\text{x}10^{-03} + 3.410\text{x}10^{-05} * \log_2(p)$	1.641x10...	0.568	1.365	0.014
	MPI_Waitall		0.157	1.788x10...	1	2.934	$3.950\text{x}10^{-03}$
	MPI_Allgather		$0.018 + 1.218\text{x}10^{-09} * p^{7/4}$	9.760x10...	0.980	5.835	0.058
	MPI_Reduce		$2.513\text{x}10^{-04}$	1.119x10...	1	13.626	0.261
	MPI_Allreduce		$0.170 + 2.478\text{x}10^{-04} * p^{1/3} * \log_2(p)$	7.463x10...	0.790	5.390	0.054
	MPI_Irecv		$2.105\text{x}10^{-03} + 5.098\text{x}10^{-05} * \log_2(p)$	2.552x10...	0.693	2.447	0.025
	MPI_Allgatherv		$3.555\text{x}10^{-04} + 2.418\text{x}10^{-07} * p^{5/4}$	2.974x10...	0.997	6.479	0.068
	▸ ComputeCornerForces		$0.089 - 1.645\text{x}10^{-04} * \log_2(p)$	1.201x10...	-0.124	0.469	$4.685\text{x}10^{-03}$
	▾ main		2.140	4.007x10...	1	1.264	$6.078\text{x}10^{-03}$
	MPI_Comm_rank		$0.013 - 1.971\text{x}10^{-05} * \log_2(p)$	9.469x10...	0.319	0.280	$2.799\text{x}10^{-03}$
	MPI_Comm_size		0.016	1.771x10...	1	0.341	$5.654\text{x}10^{-04}$
			0.072	9.185x10...	1	1.582	0.012
	MPI_Waitall		0.203	0.019	1	22.235	0.239
	MPI_Isend		$0.079 + 7.508\text{x}10^{-04} * \log_2(p)$	5.459x10...	0.695	1.033	0.010
	▸ Eval_dv_dt		$13.301 + 0.190 * \log_2(p)$	0.803	0.392	2.211	0.022
	▾ ComputeCornerForces		17.295	0.038	1	0.340	$7.466\text{x}10^{-04}$
	MPI_Reduce		$0.090 + 5.990\text{x}10^{-09} * p^{5/4} * \log_2(p)$	4.877x10...	0.684	2.470	0.025
	MPI_Allreduce		1.597		1	4.829	0.084
	MPI_Finalize		2.734x10		1	28.617	0.235
	MPI_Recv		1.304x10		0.829	39.132	0.529

All ☑ Show model ☐ Show parameters

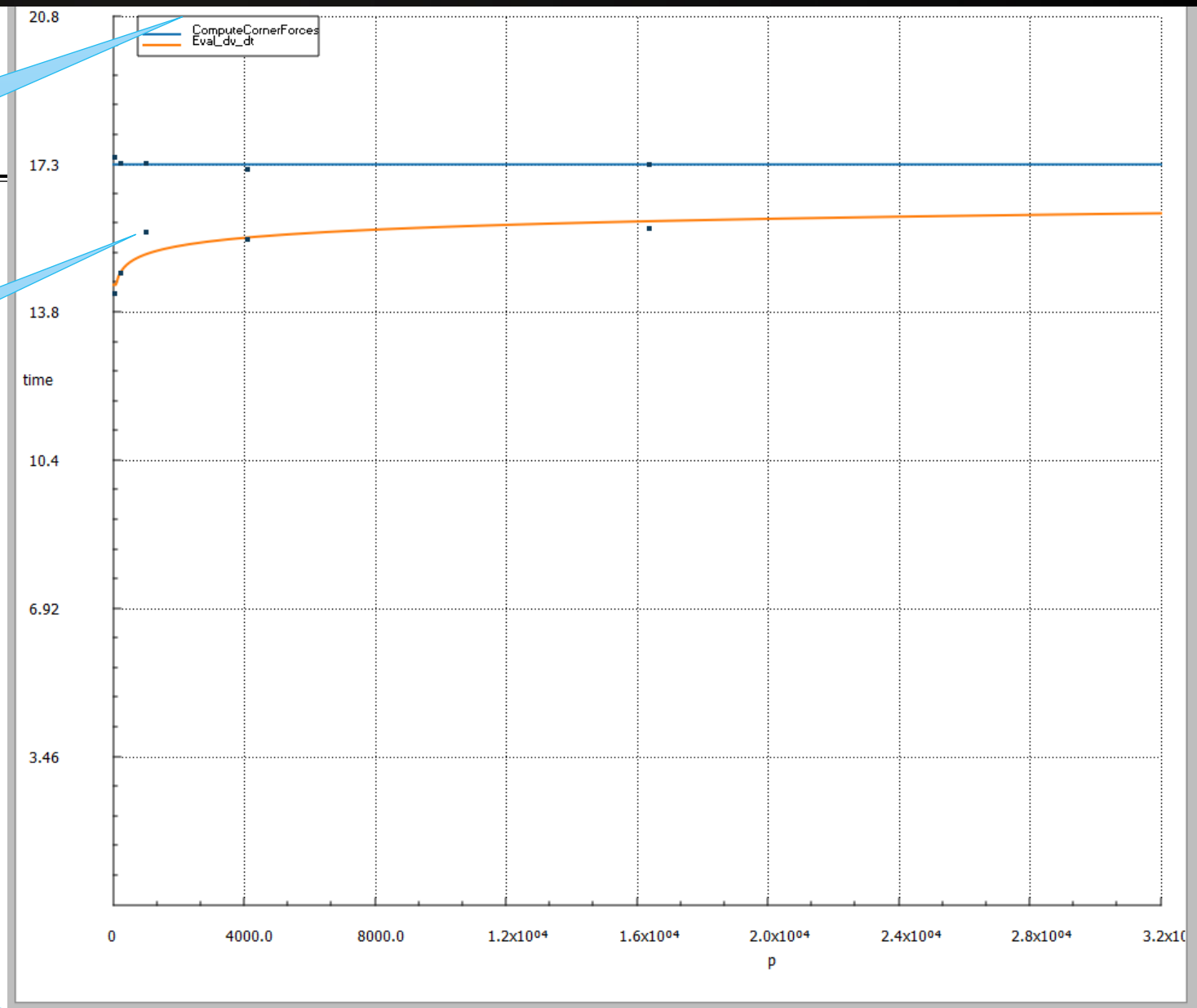
p 747

Extra-P model view

Models selected in the Call path view

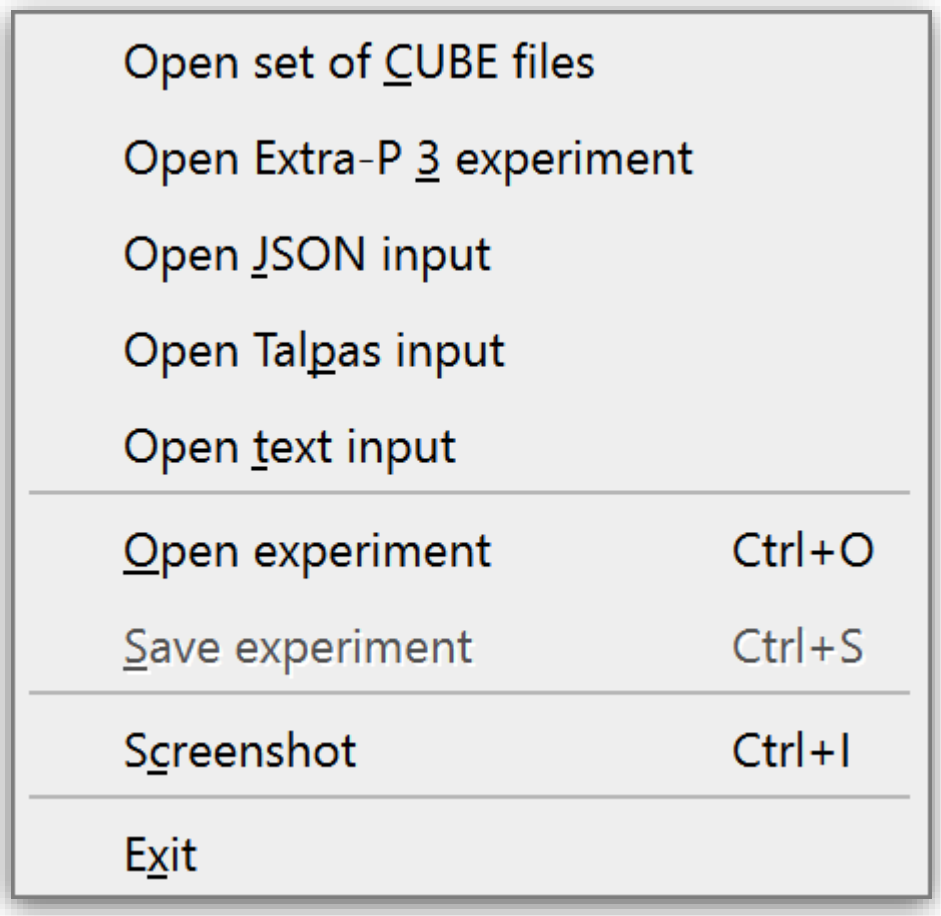
Measurement values

X axis scale control for prediction of behavior at other process counts



Modeling measurements from a text file

Choose input file



Select input file in the GUI

Extra-P input in text form

- Useful when no CUBE files are available or when modeling a small data set

```
PARAMETER p
POINTS 1000 2000 4000 8000 16000
METRIC metric1
REGION region1
DATA 1 1 1 1 1
DATA 4 4 4 3.99 4.01
DATA 16 15.999 16.01 16.01 15.99
DATA 64 64 64 64.01 63.99
DATA 256.01 255.99 256 256
```

Parameter name
This name will be used in the GUI as well as in the textual output

Measurement points
Use at least 5, but in general the more the better

Metric name

Region name
Both used to determine the output Cube file hierarchical structure and identify separate data sets

Data points
Each row corresponds to a point; all values in a row are considered repeat measurements of the same experiment

Extra-P input as JSON lines

- Useful when you do not want to use CUBE files
  - Easy to generate with your own scripts
- Each line of the file is a JSON object
  - Describes one measurement value

```
{"params": {"<parameter1>": 0, "…": "…"}, "value": 0.0,
"callpath": "<callpath>", "metric": "<metric>" } ↲
```

One line

Example

```
{"params":{"x":1,"y":1}, "metric":"metr", "callpath":"test", "value":2.03}
{"params":{"x":1,"y":2}, "metric":"metr", "callpath":"test", "value":3.02}
{"params":{"x":1,"y":3}, "metric":"metr", "callpath":"test", "value":4.01}
{"params":{"x":1,"y":4}, "metric":"metr", "callpath":"test", "value":5.02}
{"params":{"x":1,"y":5}, "metric":"metr", "callpath":"test", "value":6.01}
[…]
```

Using the command line tool

Extra-P command line tool

- Provides the same functionality, without visualization for use on cluster
- Usage guideline and command can be found at: https://github.com/extra-p/extrap

- 1.) Run: `extrap`

- Command Format: `extrap OPTIONS (--cube | --text | --talpas | --json | --extra-p-3) FILEPATH`

- 2.) Select input type: `extrap --text /lrz/sys/courses/vihps/material/extrap_data/input.txt`

Extra-P command line tool

- 3.) Output:

```
Callpath: compute
        Metric: time
                Measurement point: (2.00E+01) Mean: 8.19E+01 Median: 8.20E+01
                Measurement point: (3.00E+01) Mean: 1.79E+02 Median: 1.78E+02
                Measurement point: (4.00E+01) Mean: 3.19E+02 Median: 3.19E+02
                Measurement point: (5.00E+01) Mean: 5.05E+02 Median: 5.06E+02
                Measurement point: (6.00E+01) Mean: 7.25E+02 Median: 7.26E+02
                Model: -0.8897934098062804 + 0.20168243826499183 * x^(2)
                RSS: 3.43E+01
                Adjusted R^2: 1.00E+00
```

Callpath, kernel of the application that was measured

Metric name; either Score-P metrics (time, bytes, etc.) or custom metrics

Measurements for each input element (e.g., #processes)

Best-fit model

RSS: Residual sum of squares

Adjusted R^2 (explained previously)

Hands-on exercises

Slides are in the Extra-P material folder

- /lrz/sys/courses/vihps/2024/material/extrap/Extra-P Training.pdf

Extra-P exercises

- Install Extra-P: `pip install extrap –upgrade --pre`
- Run: `extrap`
- Example data: /lrz/sys/courses/vihps/2024/material/extrap
- Open the examples in the GUI: `extrap-gui`
- Use the command line tool: `extrap`
- Open some examples via the command line
- Produce textual output and inspect it

To get the beta version

`--help` gives an overview of the options

Extra-P on the cluster (COMMAND LINE ONLY)

- Set up environment

```
ml python/3.8.11-extended
source /lrz/sys/courses/vihps/2024/tools/extrap/venv/bin/activate
```

- Run extrap

```
extrap
```

From measurement to model

- Let's use the NAS Parallel Benchmark from earlier again

```
cd $HOME/tw45/NPB3.3-MZ-MPI/bin.scorep
```

- Reload the modules if needed

```
module load intel intel-mpi/2019-intel nano
```

- Add a new folder since you will create a lot of files

```
mkdir modeling
cd modeling
```

- We will scale the number of processes from 28 to 56 in steps of 7 processes.
  - Which type of scaling is that?

From measurement to model II-A

- Prepare a new sbatch script

```
cp /lrz/sys/courses/vihps/2024/material/extrap/measuring/modeling.sbatch .
```

```
#!/bin/bash
#SBATCH -o bt-mz.%j.out
#SBATCH -e bt-mz.%j.err
#SBATCH -J bt-mz
#SBATCH --clusters=cm2_tiny
#SBATCH --partition=cm2_tiny
#SBATCH --reservation=hhps1s24
#SBATCH --nodes=2
#SBATCH --ntasks=§NTASKS§
#SBATCH --ntasks-per-node=14
#SBATCH --get-user-env
#SBATCH --time=00:05:00
#SBATCH --array=1-4
```

From measurement to model II-B

```
module use /lrz/sys/courses/vihps/2024/modulefiles/
module load scorep/8.4-intel-intelmpi
export OMP_NUM_THREADS=4

# Score-P measurement configuration
export SCOREP_EXPERIMENT_DIRECTORY=scorep_bt-mz_sum.p§NTASKS§.r${SLURM_ARRAY_TASK_ID}
export SCOREP_FILTERING_FILE=../../config/scorep.filt

# Benchmark configuration (disable load balancing with threads)
export NPB_MZ_BLOAD=0
PROCS=28
CLASS=C

# Run the application
mpiexec -n $SLURM_NTASKS ../bt-mz_$CLASS.$PROCS
```

From measurement to model III

- You need to start the SBATCH script for the different numbers of processes

```
cp /lrz/sys/courses/vihps/2024/material/extrap/measuring/modeling.sbatch.run.sh .
```

- Make it executable and run it

```
chmod +x modeling.sbatch.run.sh
./modeling.sbatch.run.sh
```

```
#!/bin/bash
ntasks=( 28 35 42 49 56 )
for i in "${ntasks[@]}"
do
  echo "Start $i tasks"
  sed "s/§NTASKS§/$i/" modeling.sbatch > batch.tmp
  sbatch batch.tmp
done
```

- What additional features would you like to see?
- Did you find any bugs?

You can contact us via email: *extra-p-support@lists.parallel.informatik.tu-darmstadt.de*

Or on GitHub using the issues tool: *https://github.com/extra-p/extrap*