Autotuning multigrid parameters in the HMC on different architectures

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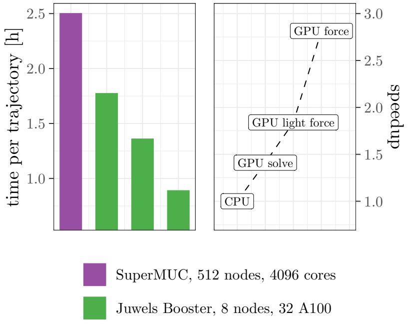
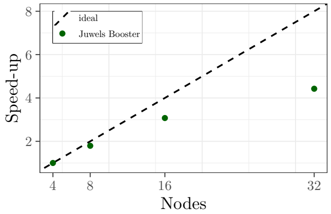
tmLQCD + QUDA

improvements over the last 18 months

$64^3 \cdot 128$ at M_π^{phys} (Juwels Booster)



Juwels Booster (A100) strong scaling



- tmLQCD: ETMC workhorse HMC implementation for $N_f = 2+1+1$ twisted mass Wilson (clover) simulations

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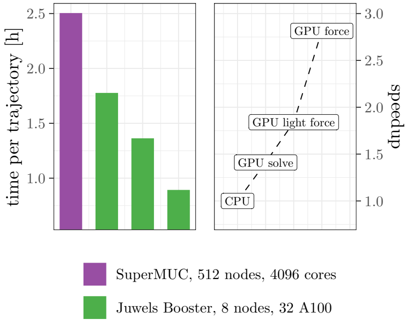

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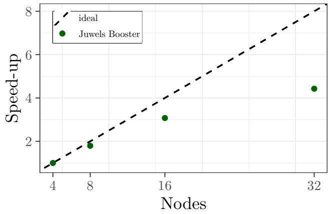

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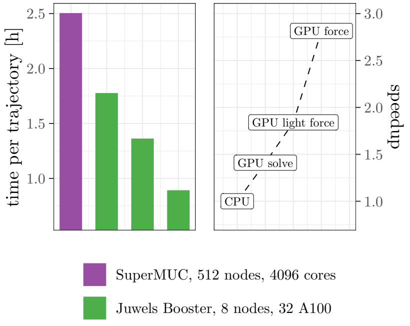

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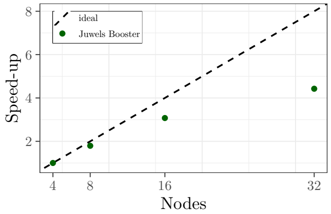

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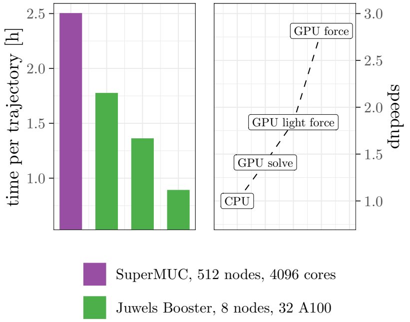

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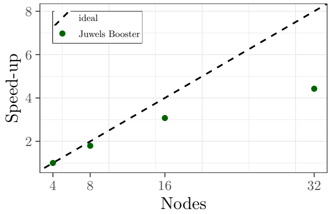

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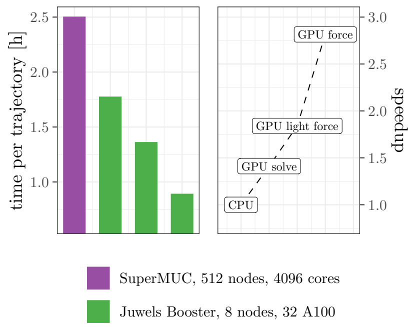

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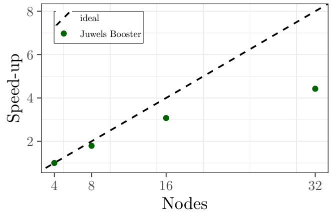

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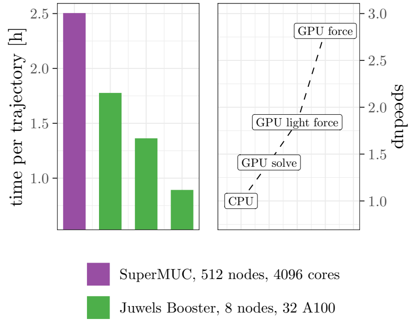

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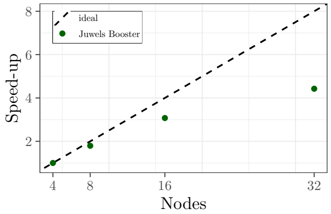

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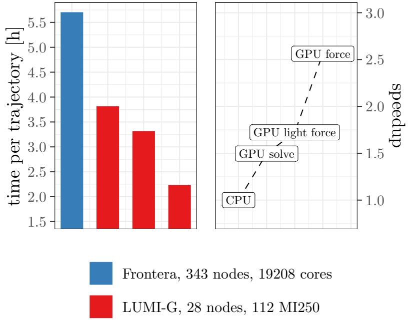
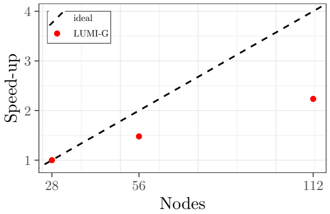
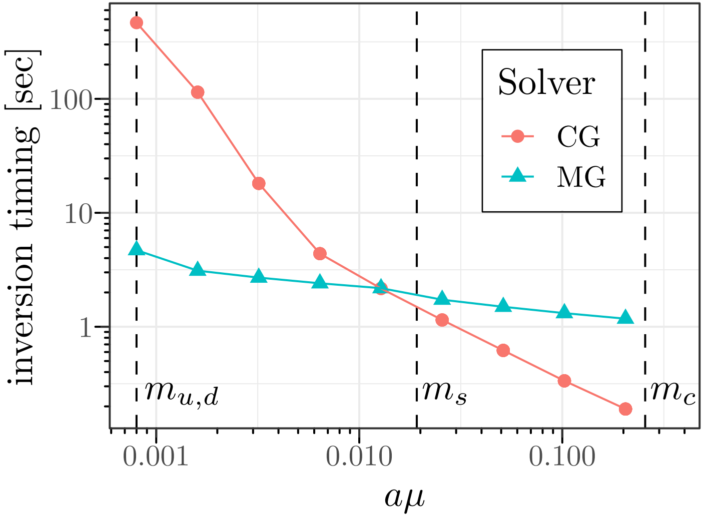
$112^3 \cdot 224$ at M_π^{phys} (LUMI-G)



LUMI-G (MI250) strong scaling



MG solver in the light sector



Comparison between MG-preconditioned-GCR
mixed-precision CG (GPU)
MG timing: two inversions + unavoidable overheads from coarse operator updates between D and $D^\dagger$ inversions

Light sector of MD Hamiltonian

In practice we employ

- 2 to 3 ρ-shifts (shifting the EO-operator)
- 3-4 time scales

$\rightarrow$ per trajectory need to solve systems with:

- $\rho = 0$ about $\mathcal{O}(100)$ times $\rightarrow$ MG
- $\rho \approx 0.001$ about $\mathcal{O}(100)$ times $\rightarrow$ MG
- $\rho \approx 0.01$ about $\mathcal{O}(200)$ times $\rightarrow$ CG
- $\rho \approx 0.1$ about $\mathcal{O}(400)$ times $\rightarrow$ CG

MG requires two solves in derivative and an update of the coarse operator (due to twisted mass sign change), but easily wins up to $\rho \approx am_s$.

Moving MG parameters from one machine to another

- Late 2022 / early 2023
  - started production of $112^3 \cdot 224$ physical point ensemble on LUMI-G (MI250)
- First computing time estimates based on performance on Juwels Booster (A100).
- Intermediate grid: $56 \cdot 4 \cdot 4 \cdot 8$ per GPU
- Coarsest grid: $8 \cdot 2 \cdot 2 \cdot 4$ per GPU
- MG parameters taken from experience

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parameter	lvl 0	lvl 1	lvl 2
`mg-mu-factor`	1.0	1.0	50.0
`mg-coarse-solver-tol`	0.1	0.1	0.1
`mg-coarse-solver-maxiter`	100	100	100
`mg-nu-post`	4	4	4
`mg-nu-pre`	2	2	2
`mg-smoother-tol`	0.1	0.1	0.1
`mg-omega`	0.9	0.9	0.9

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`mg-omega`	0.9	0.9	0.9

Juwels Booster

28 nodes: $\sim$ 6 seconds / solve

LUMI-G

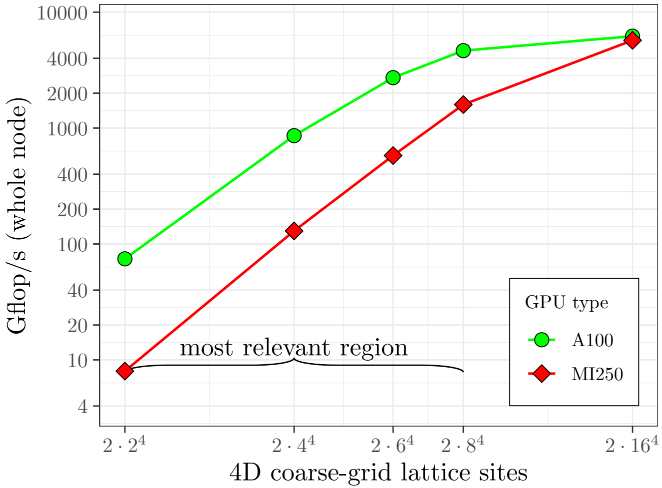
28 nodes

- **in 2023: $\sim$ 41 seconds / solve**
- today: $\sim$ 14 seconds / solve

Origin of the performance difference?

QUDA coarse-grid operator benchmark (single precision, 24 colours)

early 2023: full node (4 A100 GPUs / 8 MI250 GCDs)



- back in 2023: up to factor 6 difference in coarse-grid operator performance

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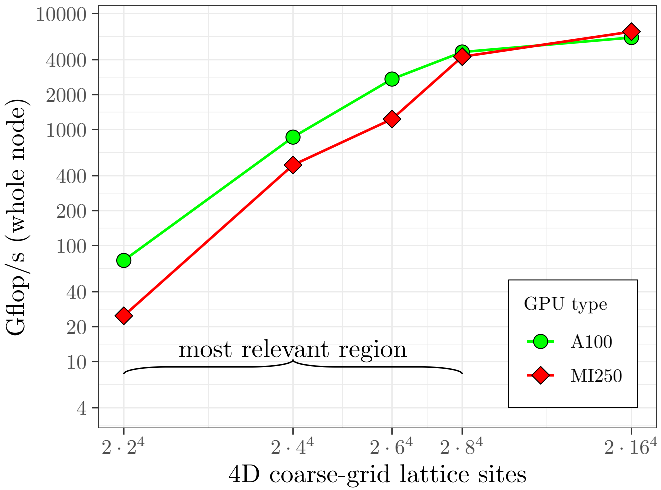

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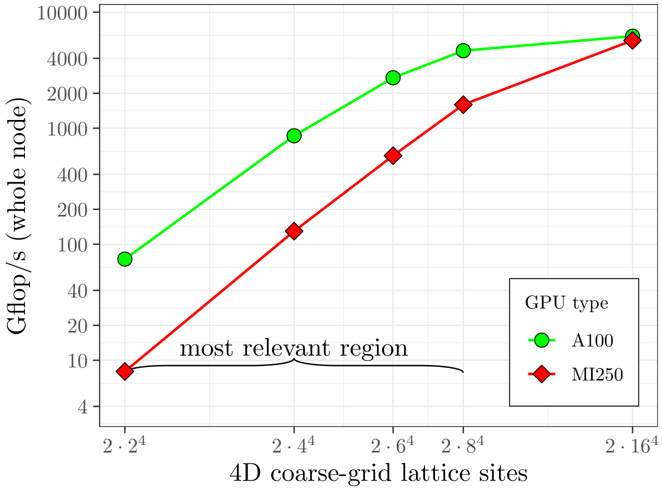

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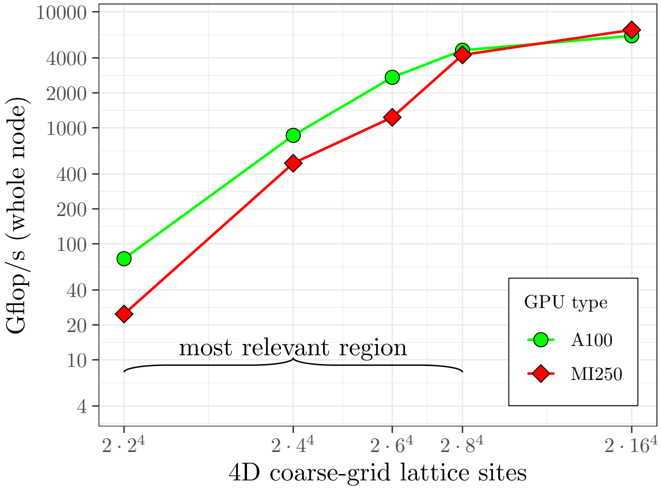

- today: down to about a factor of 2 difference

Maybe we can find a different balance between coarse, intermediate and fine iterations to obtain better performance on MI250?

Exhaustive search of MG parameters?

Parameters that can be tuned w/out redoing MG setup

parameter	sensible choices
`mg-mu-factor`	$5 \cdot 5 \cdot 15 = 375$
`mg-coarse-solver-tol`	$4^2 = 16$
`mg-coarse-solver-maxiter`	$4^2 = 16$
`mg-nu-post`	$4^3 = 64$
`mg-nu-pre`	$4^3 = 64$
`mg-smoother-tol`	$3^3 = 9$
`mg-omega`	$3^3 = 9$
total	$\approx 10^{10}$ combs

Exhaustive search of MG parameters?

Parameters which require redoing MG setup

parameter	sensible choices
`mg-block-size`	$\approx 3^2 = 9$
`mg-nvec`	$\approx 2^2 = 4$
total	≈ 36 combs

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Fully exhaustive search clearly not possible!

- fix certain params on certain levels
- do not tune less relevant params
- tune mostly / only on coarser levels

Can restrict to relevant subset of $\approx 10^6$ parameter combinations or so.

Still a major investment of computing time!

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Can we we use our intuition to find good MG setups more quickly?

“Automatic” tuning of MG parameters

https://github.com/etmc/tmLQCD/tree/deriv_mg_tune

Ideas behind proceduce:

- Always start at coarsest grid.
- Tune most relevant params first.
- Ignore small fluctuations.
- Accept even small improvements (might need several steps to see benefit).
- Tune on multiple gauge configurations.

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`mg-coarse-solver-tol`	r_0	r_1	r_2
`mg-coarse-solver-maxiter`	n_0	n_1	n_2
`mg-nu-post`	ν_0^{post}	ν_1^{post}	ν_2^{post}
`mg-nu-pre`	ν_0^{pre}	ν_1^{pre}	ν_2^{pre}
`mg-smoother-tol`	r_0^s	r_1^s	r_2^s
`mg-omega`	ω_0	ω_1	ω_2

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- **How to deal with non-converging solves?**

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`mg-nu-post`	ν_0^{post}	ν_1^{post}	ν_2^{post}
`mg-nu-pre`	ν_0^{pre}	ν_1^{pre}	ν_2^{pre}
`mg-smoother-tol`	r_0^s	r_1^s	r_2^s
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`mg-nu-post`	ν_0^{post}	ν_1^{post}	ν_2^{post}
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`mg-smoother-tol`	r_0^s	r_1^s	r_2^s
`mg-omega`	ω_0	ω_1	ω_2

repeat μ_2

Global tuning procedure parameters

- Number of tuning steps per gauge configuration, N (f.ex. 100).
- Tolerance δ: stop tuning the current parameter, f.ex. $t_i/t_{\text{best}} > 0.995$
- Threshold ρ: ignore fluctuations when choosing t_{best}, f.ex. $t_i/t_{\text{best}} > 0.999$

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`mg-nu-post`	ν_0^{post}	ν_1^{post}	ν_2^{post}
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For each parameter p on level ℓ

- maximum number of steps to be done n_p^ℓ
- change in parameter per step $\pm\Delta_p^\ell$

1 perform n_p^ℓ steps of $p^\ell + \Delta_p^\ell$, or until timing stops improving

2 if timing does not improve (or worsens), move to next p on current ℓ

3 move to next-finest level and follow same sequence

4 if step $i < N$, go back to (1)

4 if step $i = N$, move to next gauge configuration, reset $i = 0$

Tuning MG parameters for a $112^3 \cdot 224$ ensemble at M_π^{phys} (from above, LUMI-G)

tuning from above
reducing cost step-by-step

Initial parameters:

parameter	lvl 0	lvl 1	lvl 2
`mg-mu-factor`	1.0	1.0	30.0
`mg-coarse-solver-tol`	0.05	0.05	0.05
`mg-coarse-solver-maxiter`	50	50	50
`mg-nu-post`	6	6	6
`mg-nu-pre`	6	6	6
`mg-smoother-tol`	0.05	0.05	0.05
`mg-omega`	0.85	0.85	0.85

- Positive Δ for:
  - `mg-mu-factor`
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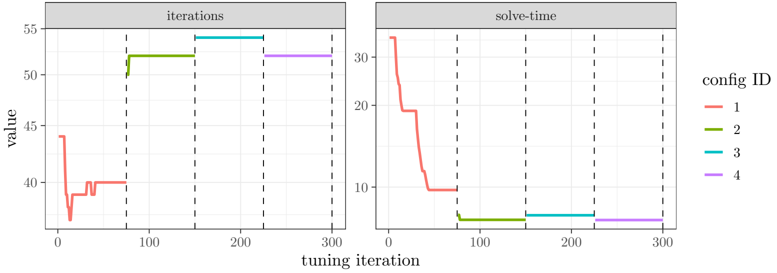

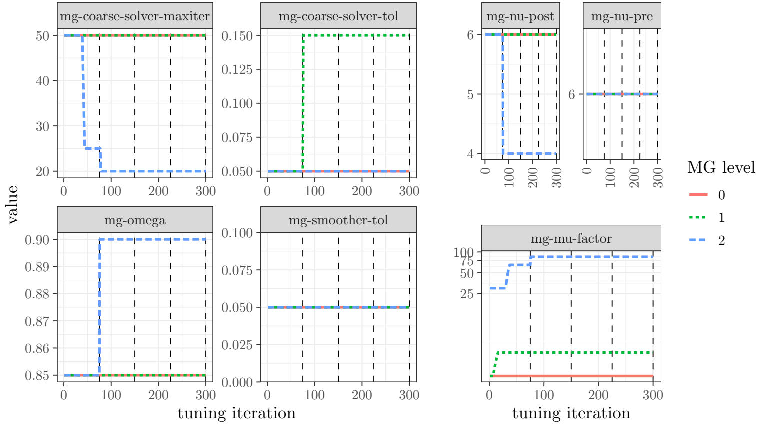

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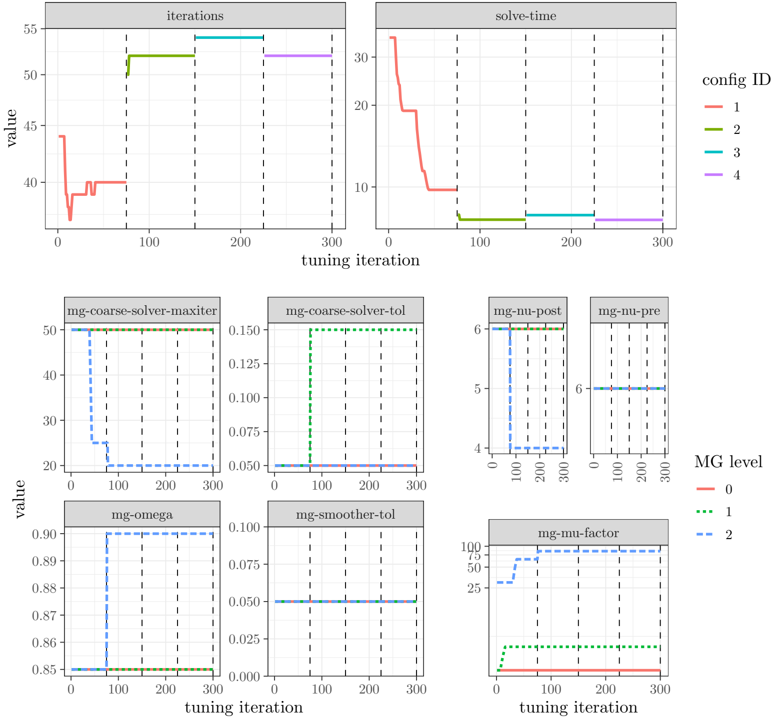

from 40+ seconds to $\sim$ 8 seconds
in a few hundred solves

Tuning MG parameters for a $112^3 \cdot 224$ ensemble at M_π^{phys} (from below, LUMI-G)

tuning from below
increasing cost step-by-step

Initial parameters:

parameter	lvl 0	lvl 1	lvl 2
`mg-mu-factor`	1.0	1.0	30.0
`mg-coarse-solver-tol`	0.55	0.55	0.55
`mg-coarse-solver-maxiter`	5	5	5
`mg-nu-post`	1	1	1
`mg-nu-pre`	1	1	1
`mg-smoother-tol`	0.55	0.55	0.55
`mg-omega`	0.85	0.85	0.85

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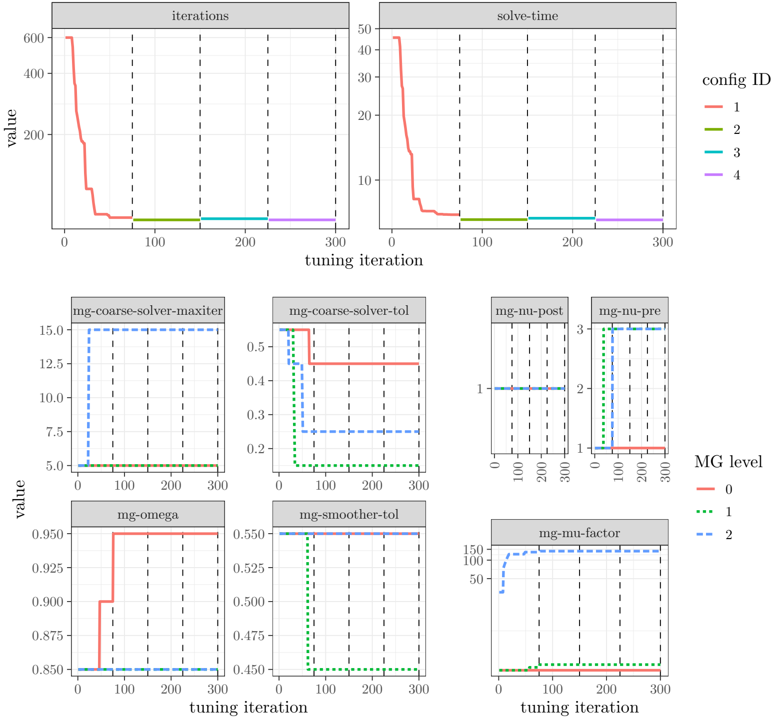
`mg-coarse-solver-tol`	0.55	0.55	0.55
`mg-coarse-solver-maxiter`	5	5	5
`mg-nu-post`	1	1	1
`mg-nu-pre`	1	1	1
`mg-smoother-tol`	0.55	0.55	0.55
`mg-omega`	0.85	0.85	0.85

- Positive Δ for:
  - `mg-mu-factor`
  - `mg-coarse-solver-maxiter`
  - `mg-nu-post`
  - `mg-nu-pre`
- Negative Δ for:
  - `mg-coarse-solver-tol`
  - `mg-smoother-tol`



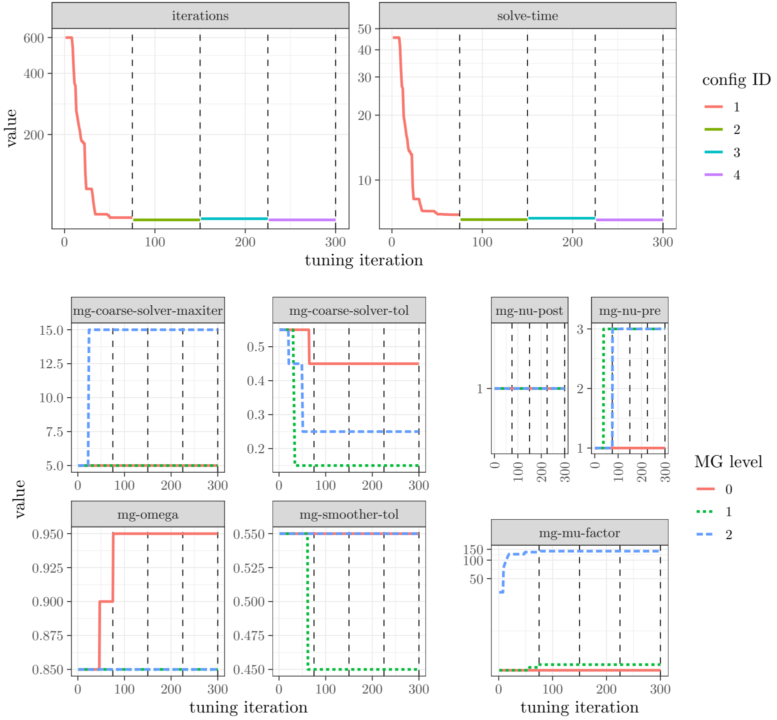
Tuning MG parameters for a $112^3 \cdot 224$ ensemble at M_π^{phys} (from below, LUMI-G)

tuning from below
increasing cost step-by-step

Initial parameters:

parameter	lvl 0	lvl 1	lvl 2
`mg-mu-factor`	1.0	1.0	30.0
`mg-coarse-solver-tol`	0.55	0.55	0.55
`mg-coarse-solver-maxiter`	5	5	5
`mg-nu-post`	1	1	1
`mg-nu-pre`	1	1	1
`mg-smoother-tol`	0.55	0.55	0.55
`mg-omega`	0.85	0.85	0.85

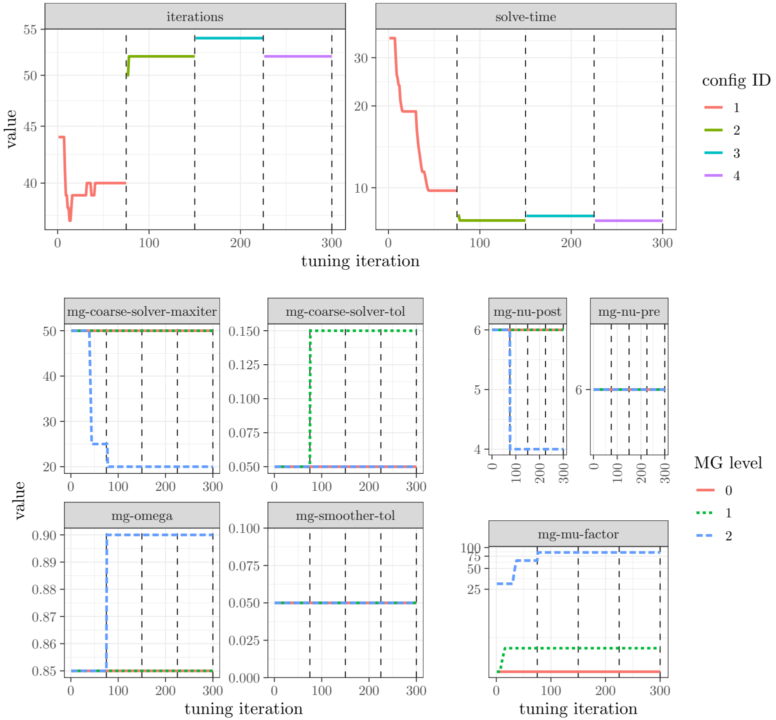
- Positive Δ for:
  - `mg-mu-factor`
  - `mg-coarse-solver-maxiter`
  - `mg-nu-post`
  - `mg-nu-pre`
- Negative Δ for:
  - `mg-coarse-solver-tol`
  - `mg-smoother-tol`



from non-convergence to $\sim$ 7 seconds
in a few hundred solves

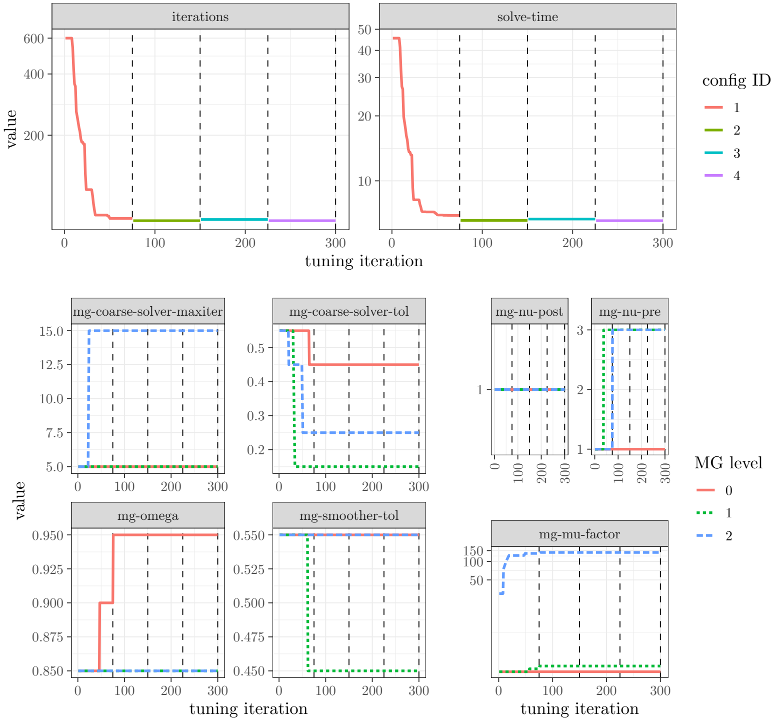
Tuning MG parameters for a $112^3 \cdot 224$ ensemble at M_π^{phys} (Comparison)

tuning from above



7.5 to 9 seconds

tuning from below



6.5 to 7 seconds

(depending on gauge configuration)

So, does it work?

Let's recall the $112^3 \cdot 224$ ensemble @ M_π^{phys} running on LUMI-G.

Juwels Booster

28 nodes

- Before tuning: $\sim$ 6 seconds / solve
- After tuning: $\sim$ 4 seconds / solve

LUMI-G

28 nodes

- Before tuning: $\sim$ 14 seconds / solve
- After tuning: $\sim$ 7 seconds / solve

So, does it work?

Let's recall the $112^3 \cdot 224$ ensemble @ M_π^{phys} running on LUMI-G.

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LUMI-G

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- After tuning: $\sim$ 7 seconds / solve

This was way more impressive back in 2023 when we went from 41 to $\sim$ 10 seconds.

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Improves setups also in situations where intuition was okay.

Finds parameters combinations that we would not have thought of.

Nice corollary: can also further improve coarse-grid-deflated solver, used to good effect on LUMI-G.

$\Rightarrow$ Useful also for measurement campaigns.

Limitations

- Not currently integrated into HMC.
  - Currently: need to prepare set of configurations and perform separate run.
  - Integration directly into HMC possible: tuner is already called from within fermionic derivative.
- Not tested on untwisted Wilson clover.
  - Should work out of the box, need gauge configs in ILDG format. (ignore `mg-mu-factor`)
- Does not tune parameters which need MG setup to be regenerated.
  - Required logic extension simple but tedious.
- Some of the parameter evolution does not seem to make a lot of sense.
  - Might require some more fine-tuned intervention logic.
- Thresholds and starting parameters can have big impact on tuning quality.
  - Need some more systematic guidelines to judge impact of lattice spacing, target quark mass and lattice volume.

Where to get it?

If you want to play around with the code:

- `https://github.com/etmc/tmLQCD/tree/deriv_mg_tune`
- `deriv_mg_tune` executable
- all input file parameters explained in documentation
- `quda_interface.c`: `quda_mg_tune_params` function (and various helper functions)

Many thanks for your attention!

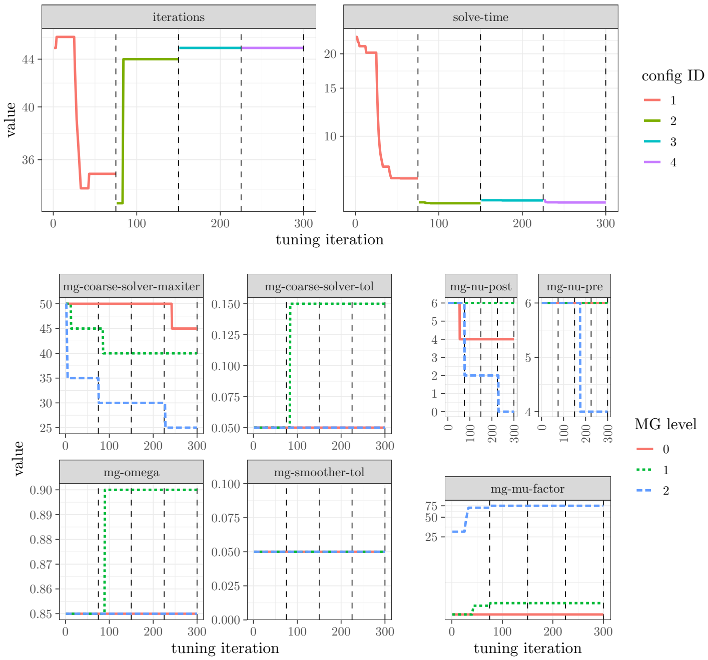
Backup

Backup Slides

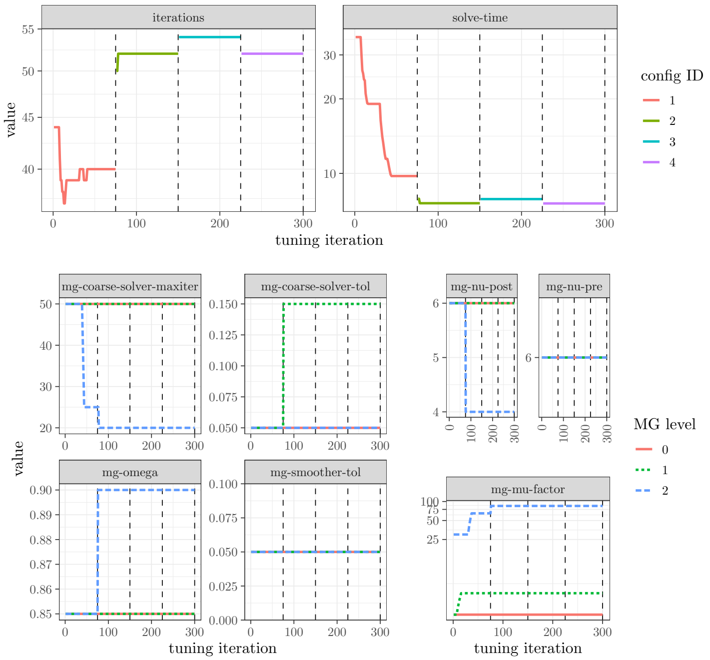
Comparison between Juwels Booster and LUMI-G

tuning from above

Juwels Booster



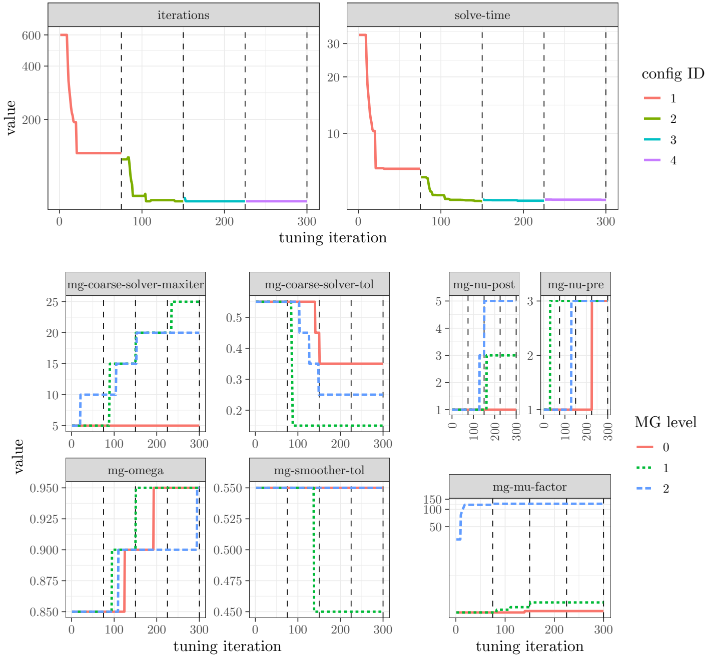
LUMI-G



Comparison between Juwels Booster and LUMI-G

tuning from below

Juwels Booster



LUMI-G