A parameter optimisation toolchain for Monte Carlo detector simulation

- improving the recipe for full detector simulations -

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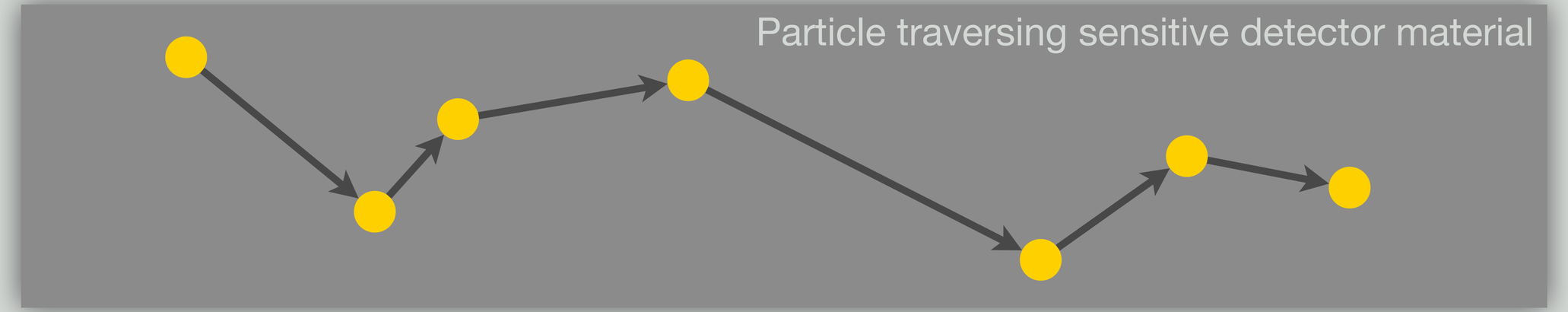
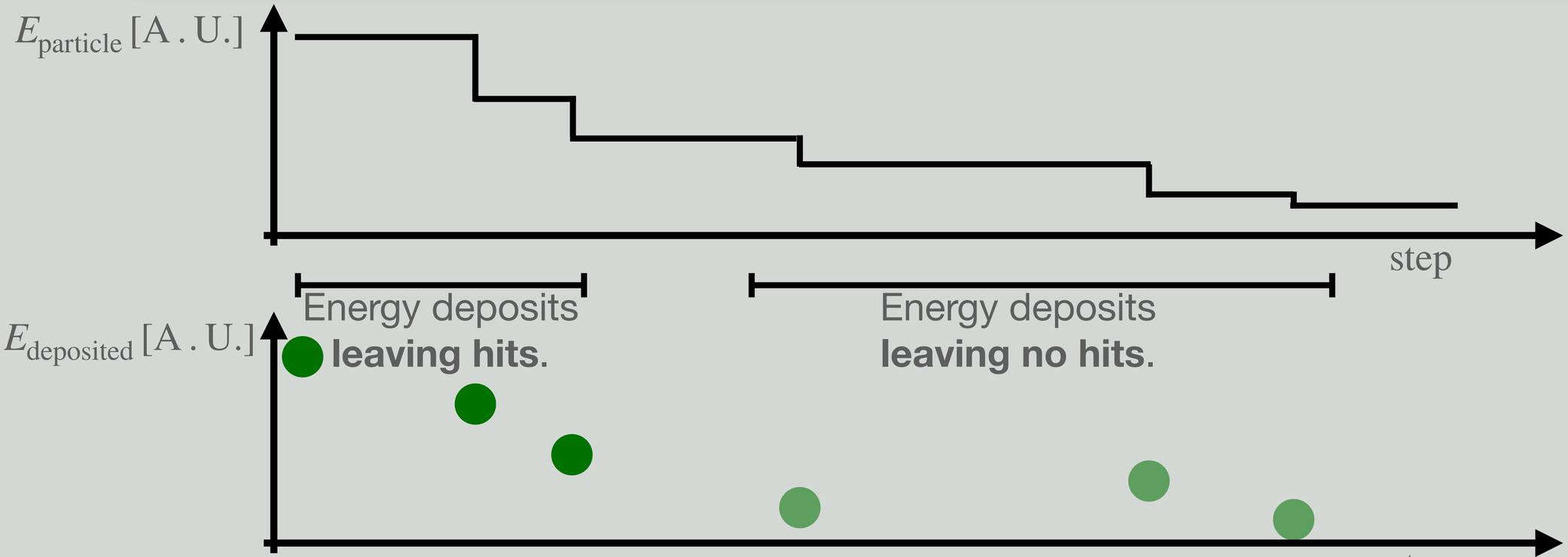
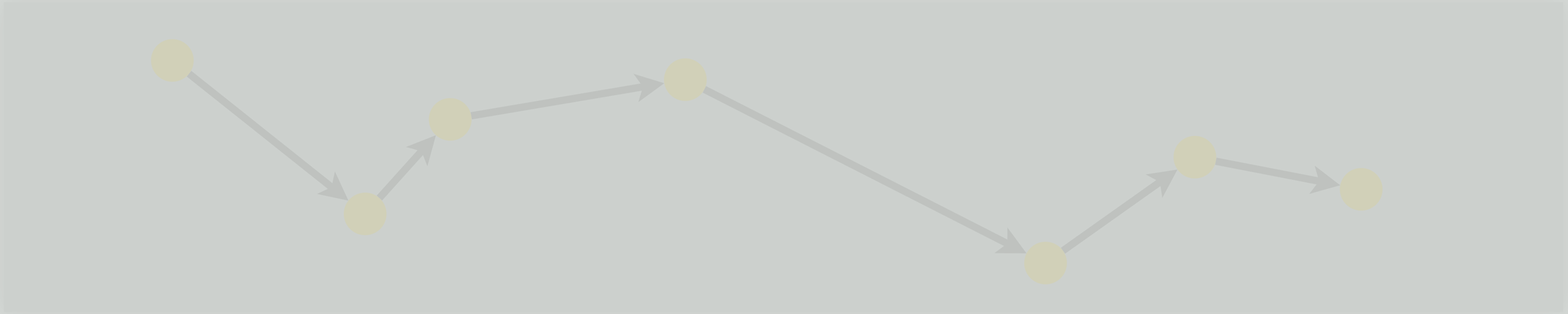
CHEP2023/Track 3 - 09.05.2023

MC transport recipe

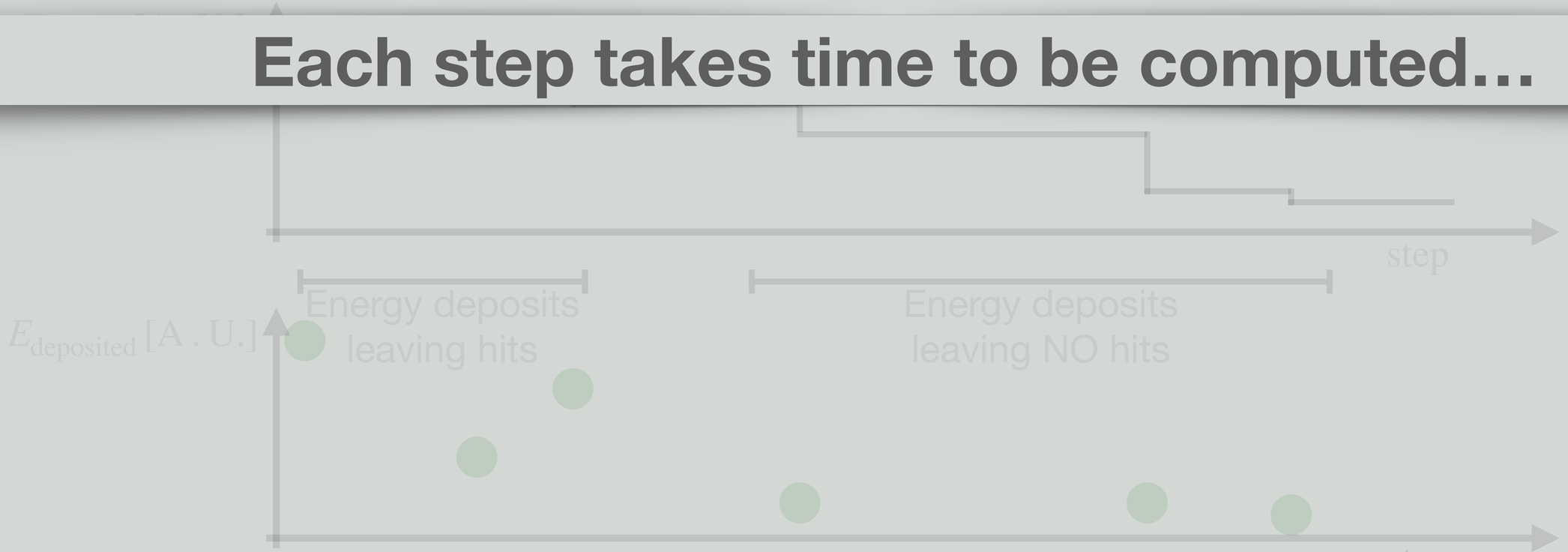




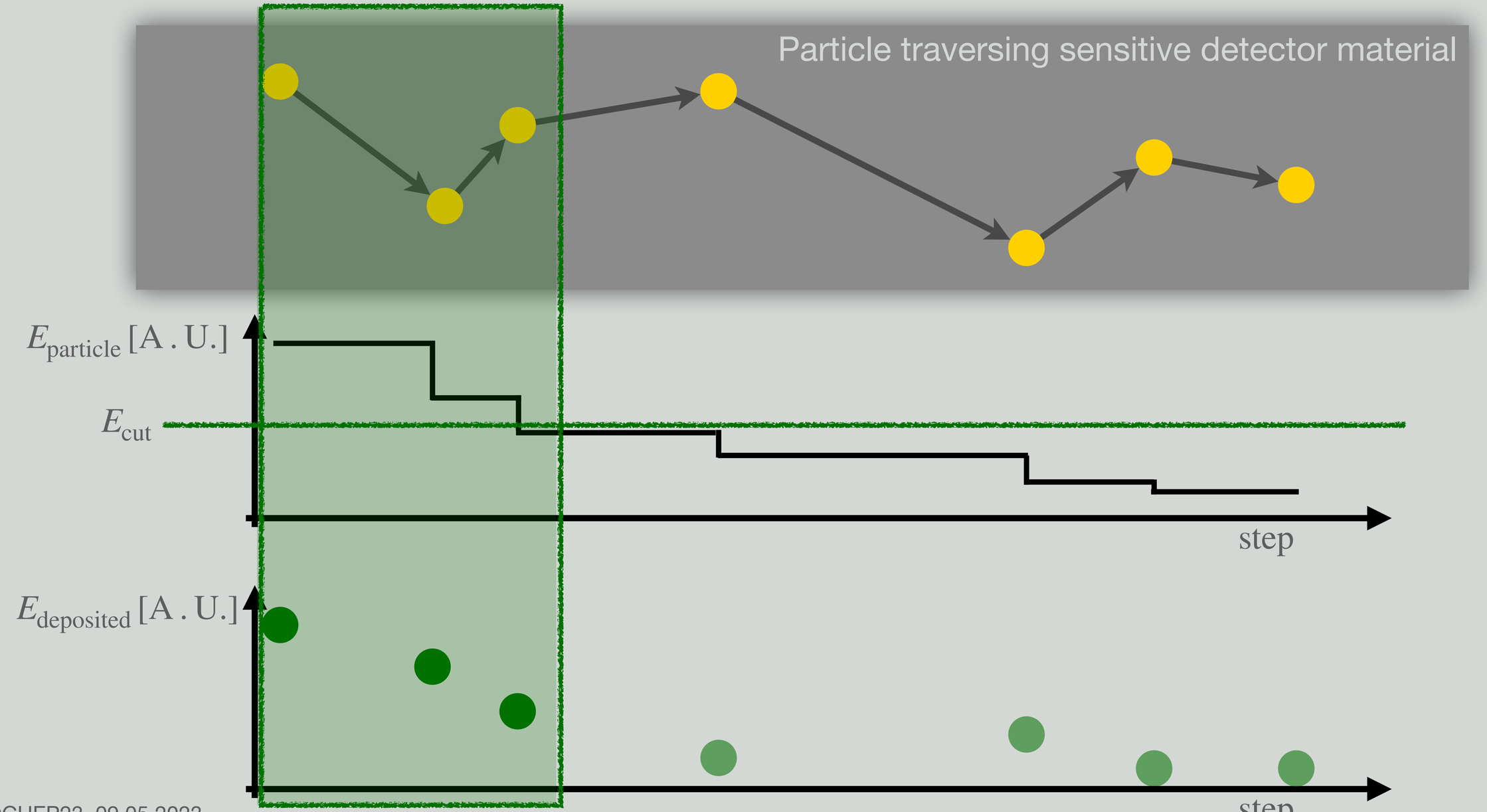
MC transport recipe



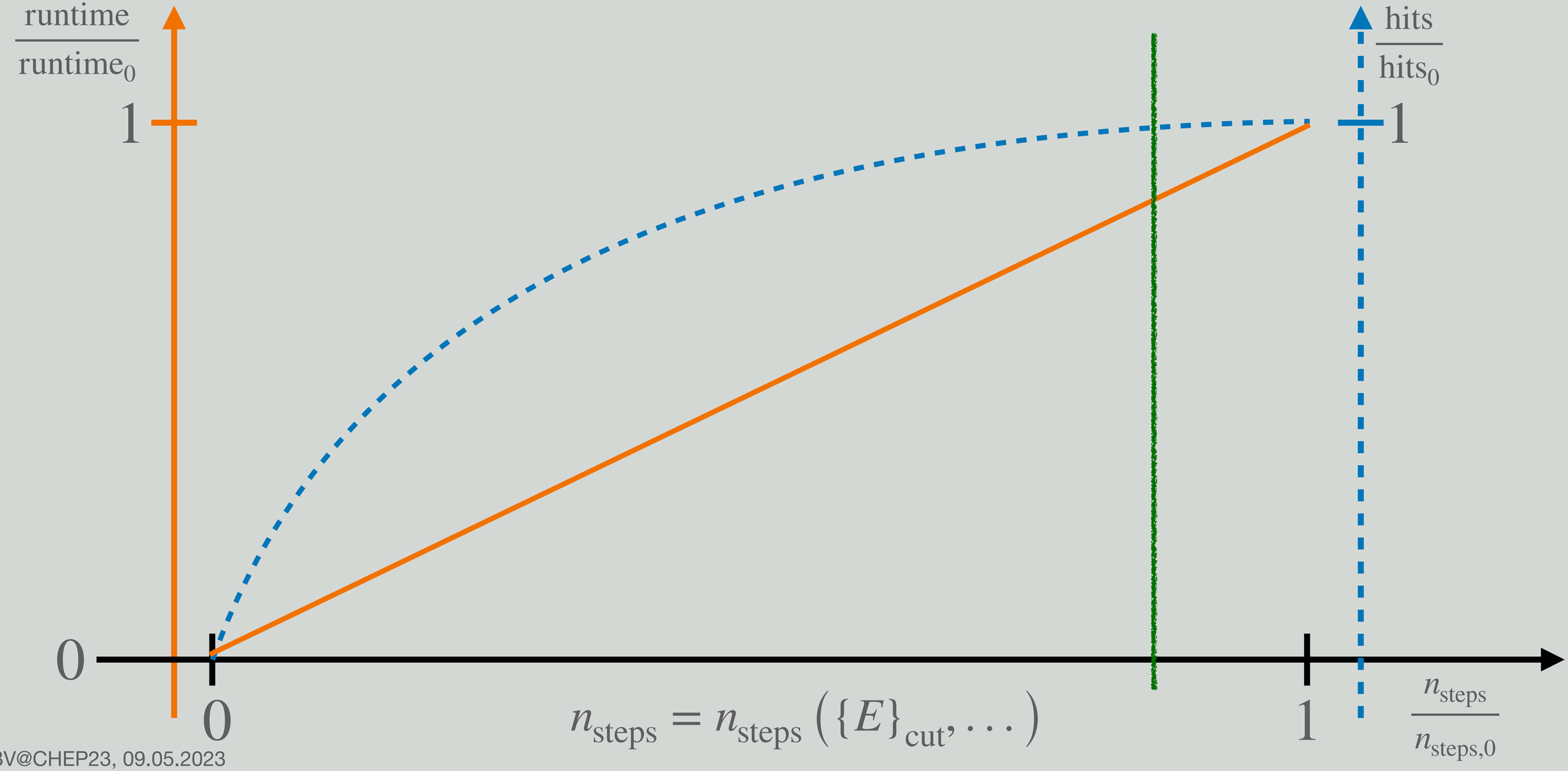
Each step takes time to be computed…



Steps without hits don’t add to the taste…



…so we might speed up the preparation!



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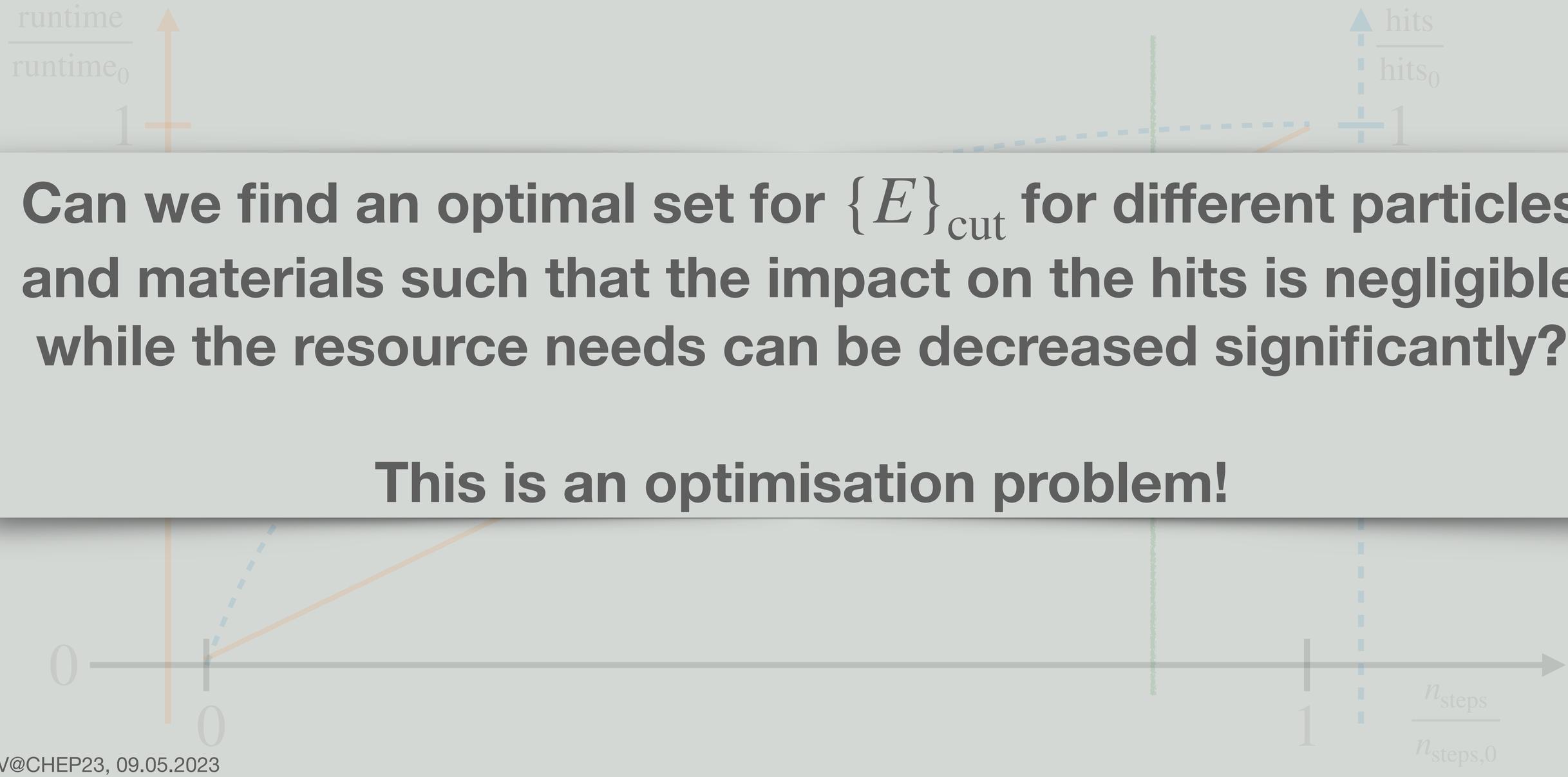
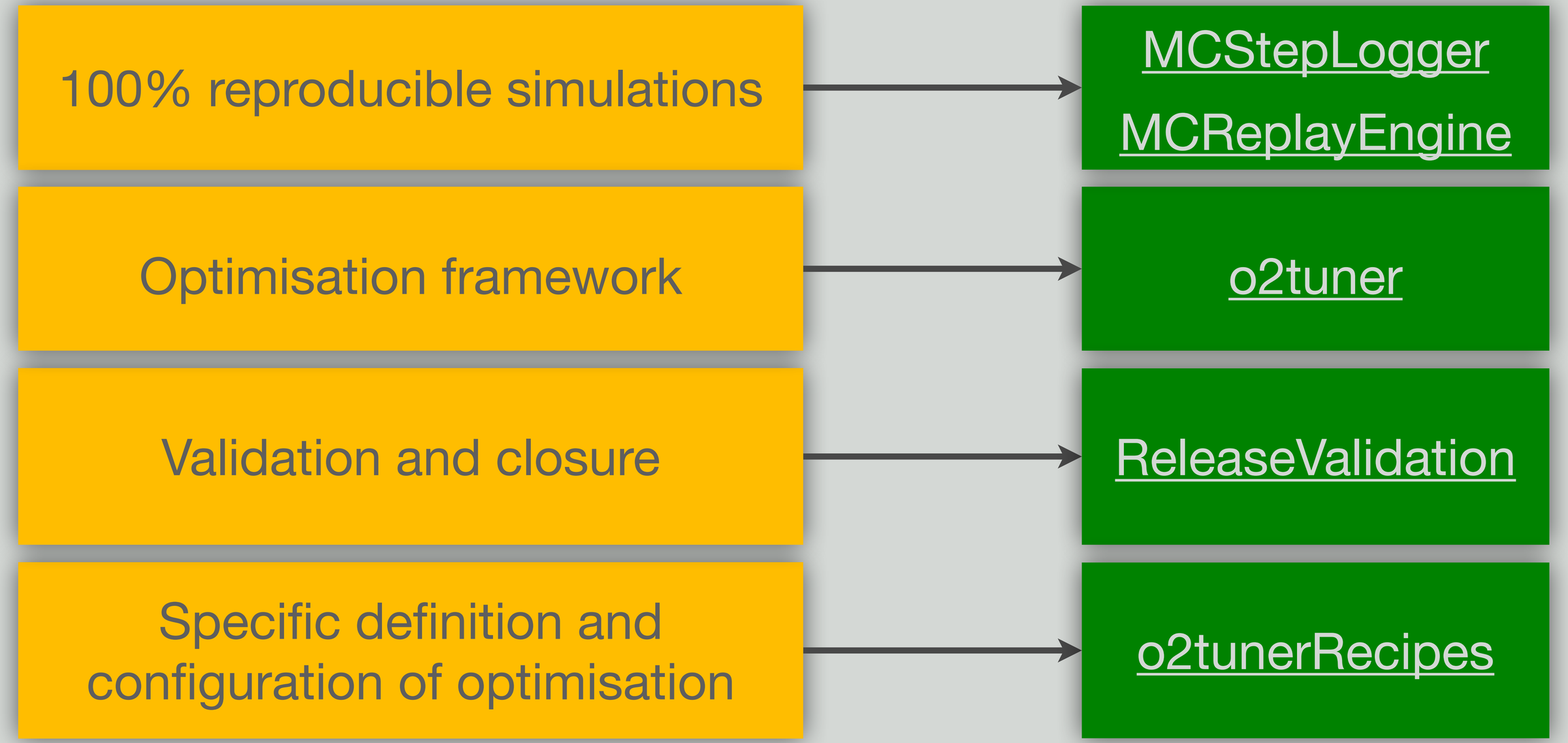


Can we find an optimal set for $\{E\}_{\text{cut}}$ for different particles and materials such that the impact on the hits is negligible while the resource needs can be decreased significantly?

This is an optimisation problem!

Ingredients

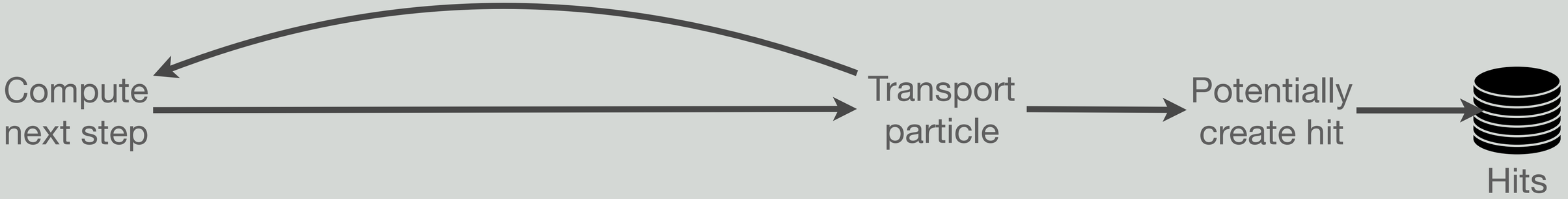


Ingredients - precooked

100% reproducible simulations

MCStepLogger

MCReplayEngine



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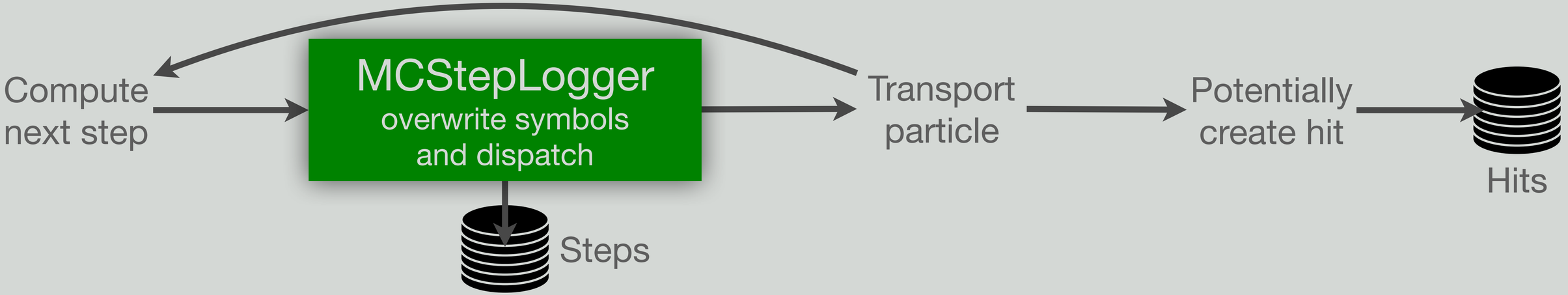

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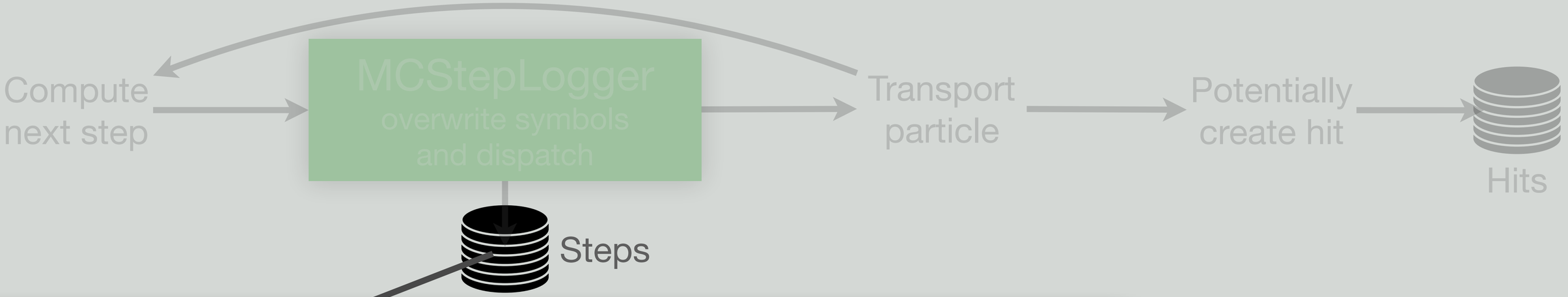
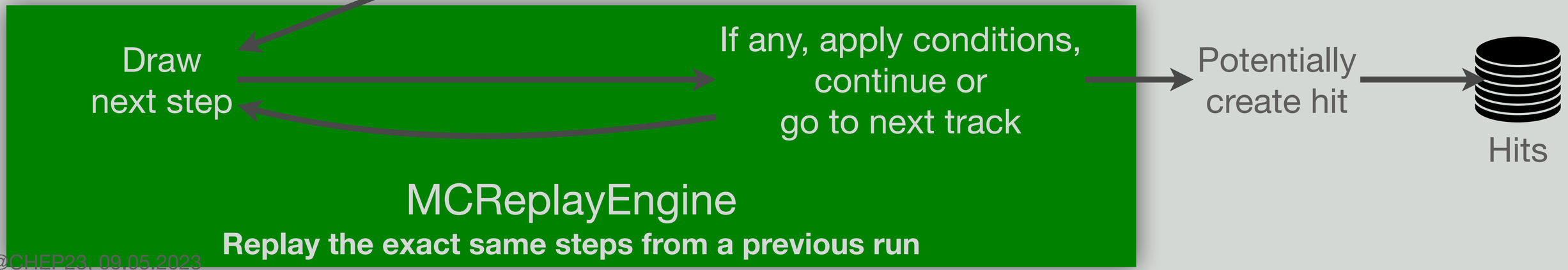
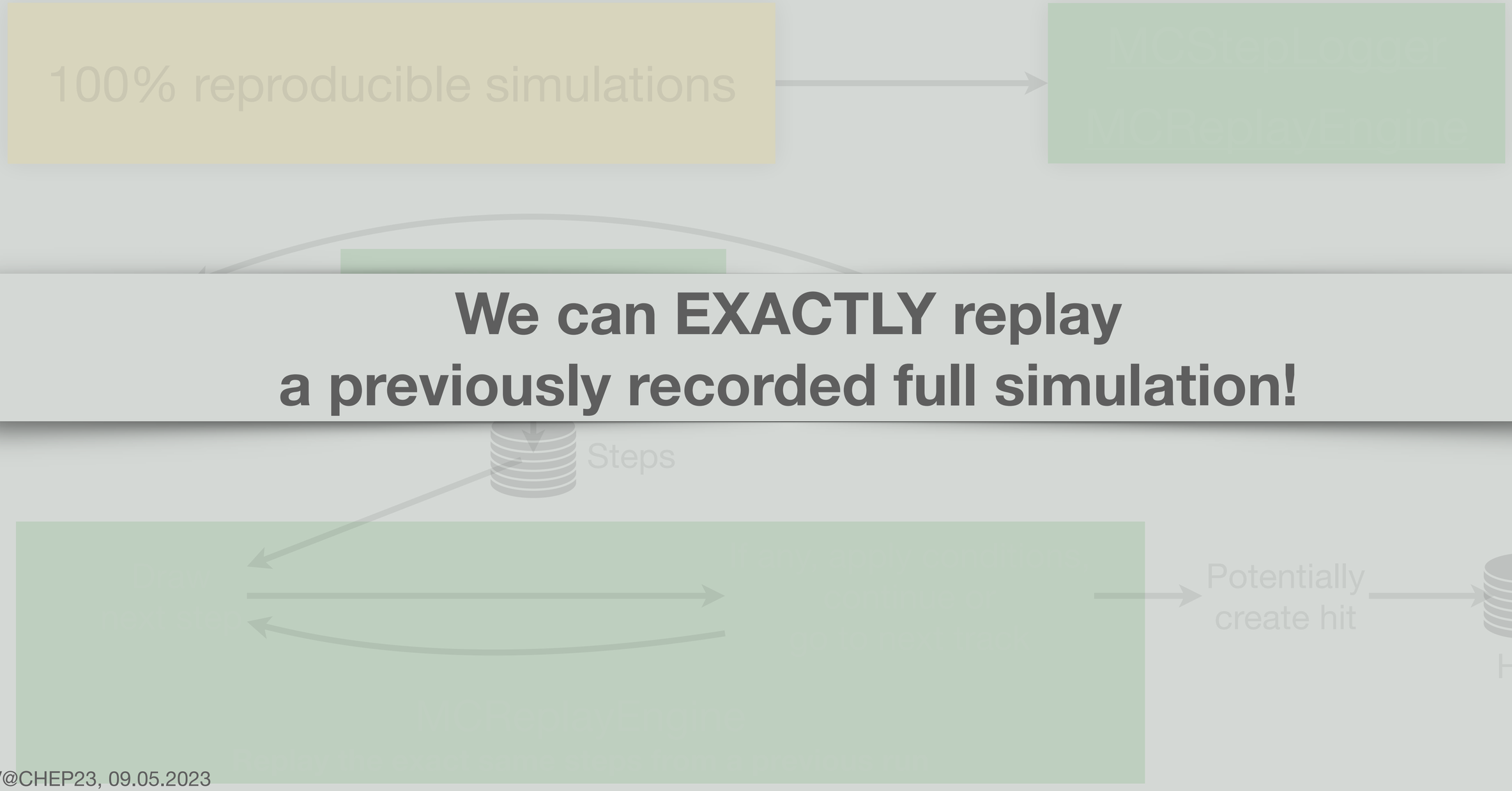




Ingredients - precooked



We can EXACTLY replay
a previously recorded full simulation!

Ingredients - precooked

- Execute user-defined recipe
  - Work through necessary steps (e.g. data preparation, optimisation, evaluation)
  - Ensure reproducibility
  - Wrap parallelisation
  - **Optimise** various applications such as ML models or **parameter-dependent executables and scripts**

Ingredients - precooked

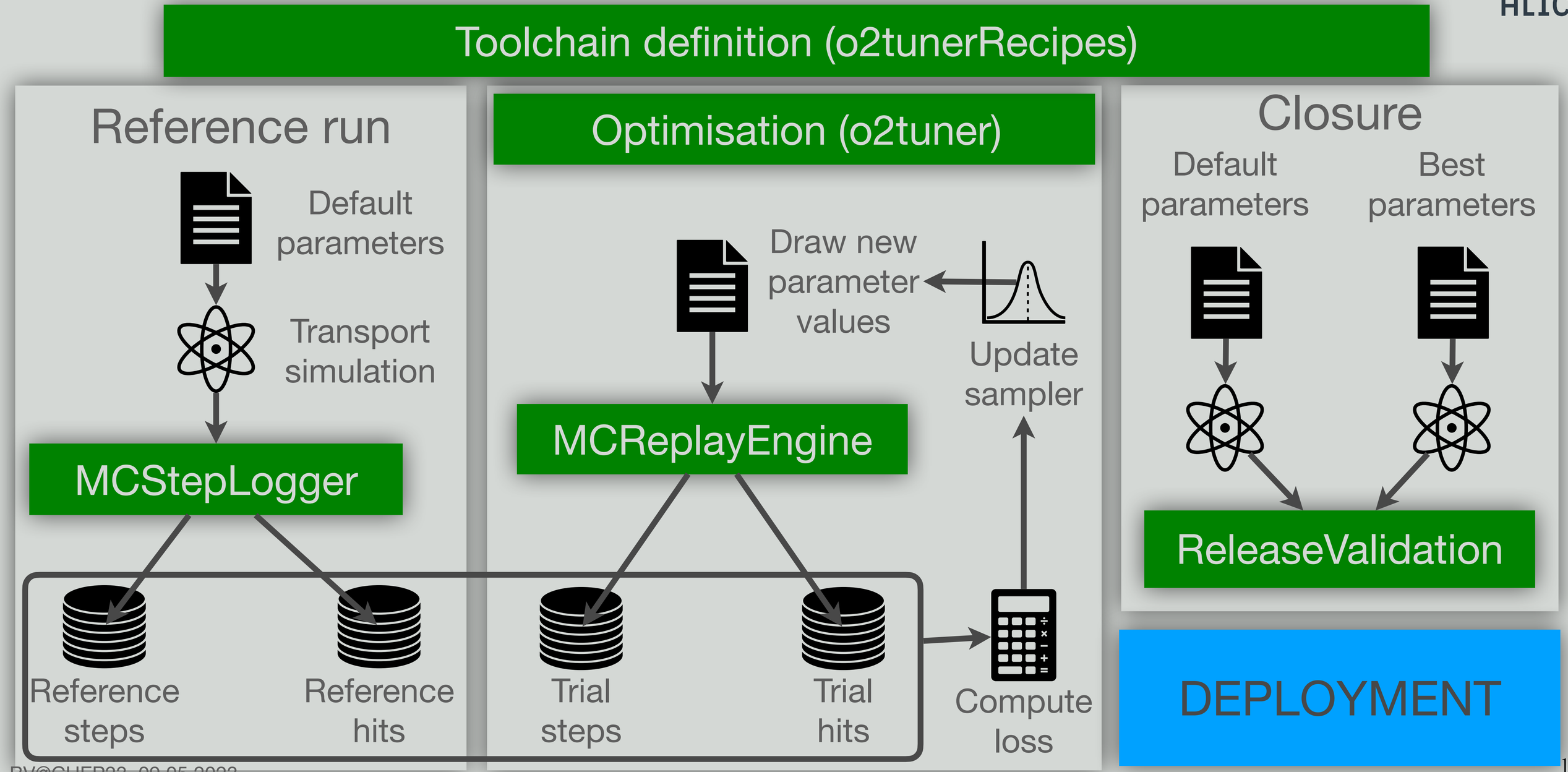
- Automatically
  - Compare various different observables
  - Compute various different metrics
  - Plot and report summaries

Ingredients - prepared by the user

Specific definition and configuration of optimisation → o2tunerRecipes

- Toolchain definition
  - Objective function and loss [required]
  - Functions for (reference) data creation [optional]
  - User-defined evaluation and closure tests [optional]
  - Optimisation configuration [optional]
    [number of trials, jobs, parameter sampling etc.]

Preparation



Pre-cook the loss

Steps themselves are **invisible** to the detectors. They are the results of MC calculations.

Hits are the physical energy deposits a detector **can see**. This is what we need to keep.

Keep hits while dropping steps! Defining the loss.

Pre-cook the loss

Steps ⟶ Hits

$$\frac{\partial L}{\partial s_{\mathrm{t}}} > 0 \qquad \frac{\partial L}{\partial h_{\mathrm{t}}^{\mathrm{d}}} < 0$$

Define a metric to be evaluated for each chosen set of drawn values.

$$L_{\mathrm{t}}\left(s_{\mathrm{ref}}, \{h\}_{\mathrm{ref}}^{\mathrm{d}}, s_{\mathrm{t}}, \{h\}_{\mathrm{t}}^{\mathrm{d}}\right) =$$

Optimisation trial t,
Number of steps s,
Detector d,
Hits h^{d} in detector,
detector-specific penalty α^{d}.

Pre-cook the loss

Steps ⟶ Hits

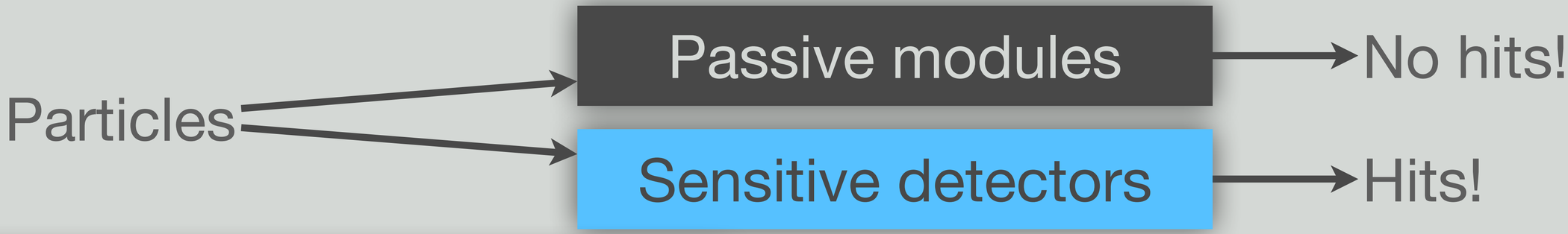
$$\frac{\partial L}{\partial s_\mathrm{t}} > 0 \qquad \frac{\partial L}{\partial h_\mathrm{t}^\mathrm{d}} < 0$$

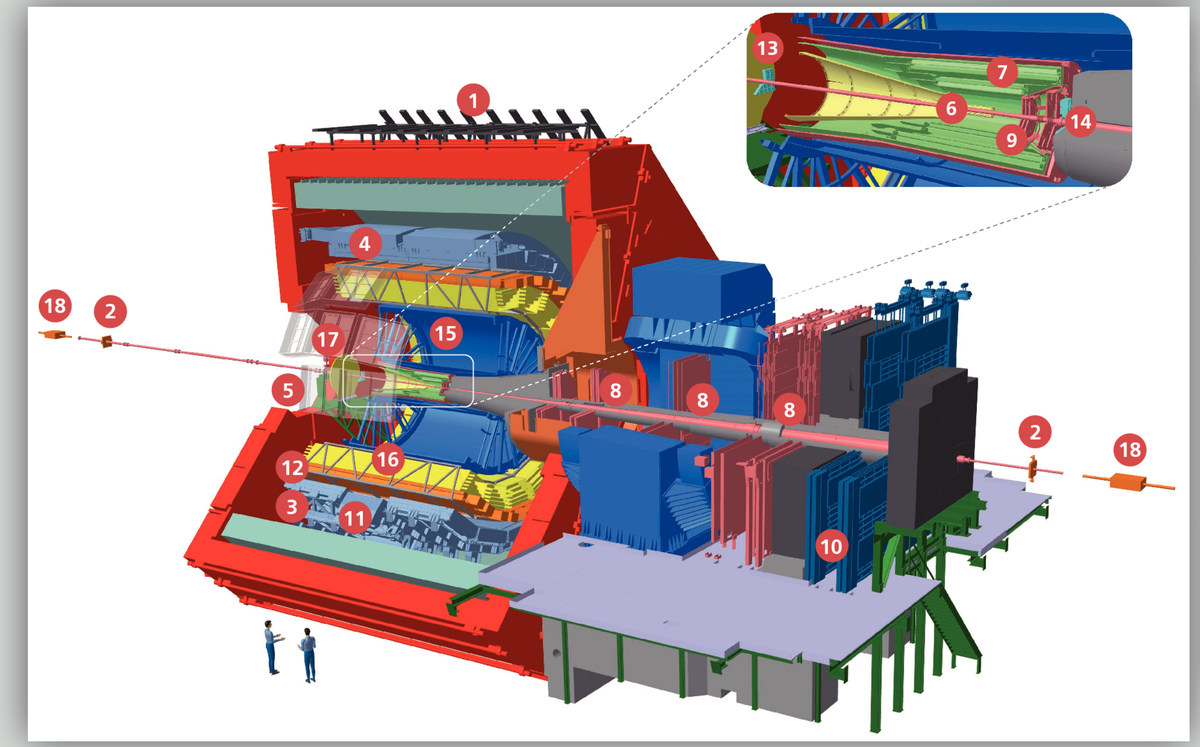
Define a metric to be evaluated for each chosen set of drawn values.

$$L_\mathrm{t}\left(s_\mathrm{ref}, \{h\}_\mathrm{ref}^\mathrm{d}, s_\mathrm{t}, \{h\}_\mathrm{t}^\mathrm{d}\right) = \frac{s_\mathrm{t}}{s_\mathrm{ref}} + \frac{1}{N^\mathrm{det}} \sum_{\mathrm{d}\in\mathrm{det}} \alpha^\mathrm{d}\left(h_\mathrm{t}^\mathrm{d}, h_\mathrm{ref}^\mathrm{d}\right) \cdot \left[1 - \frac{h_\mathrm{t}^\mathrm{d}}{h_\mathrm{ref}^\mathrm{d}}\right]$$

Optimisation trial t,
Number of steps s,
Detector d,
Hits h^d in detector,
detector-specific penalty α^d.

Final thoughts before optimising





We first target the reduction **of steps in passive modules: only leave what will eventually be seen by detectors.**

Show results for beam pipe.

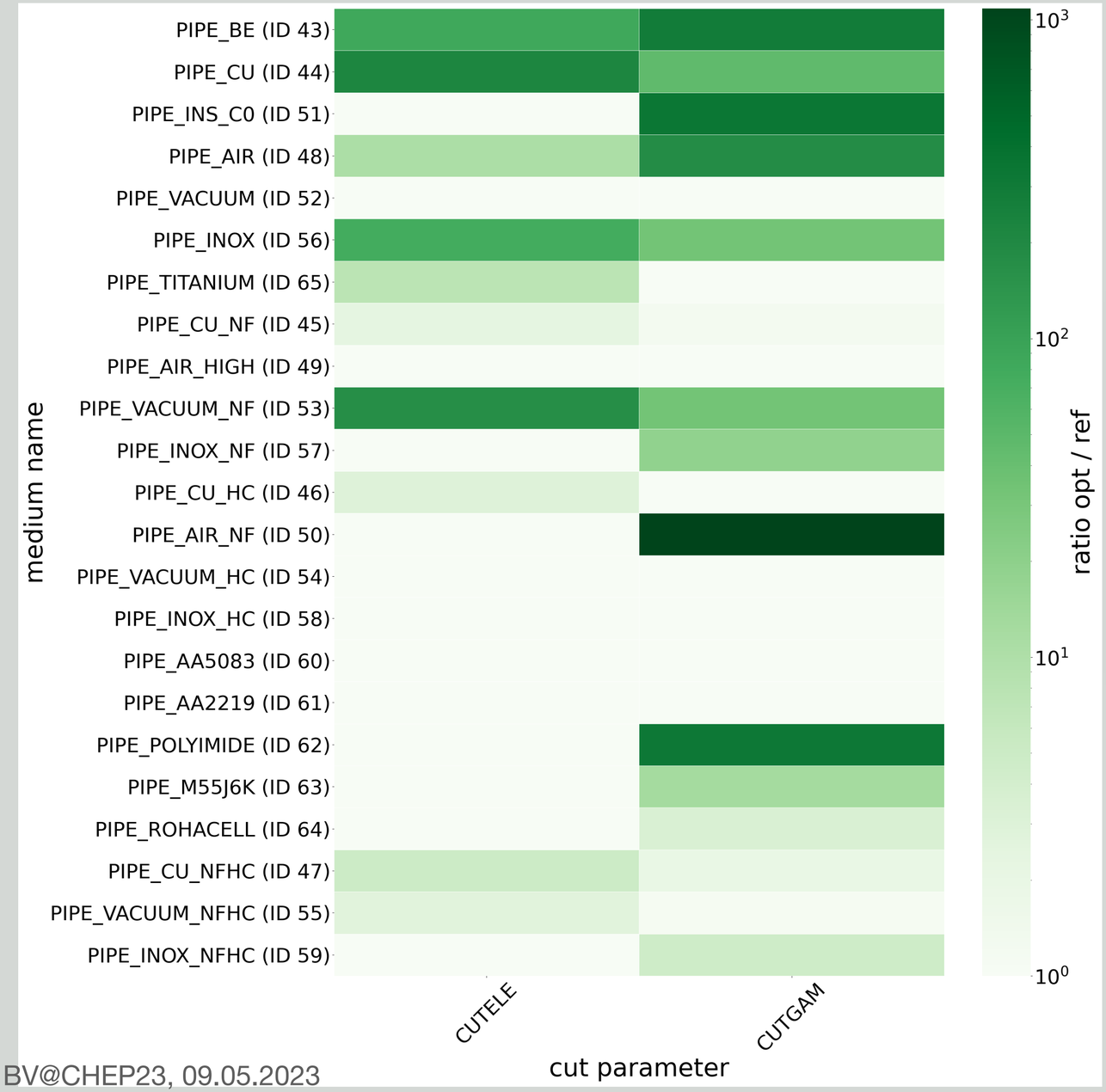
Account for hits in all detectors.

Optimisation…

boiling, waiting, stirring…

Tasting!

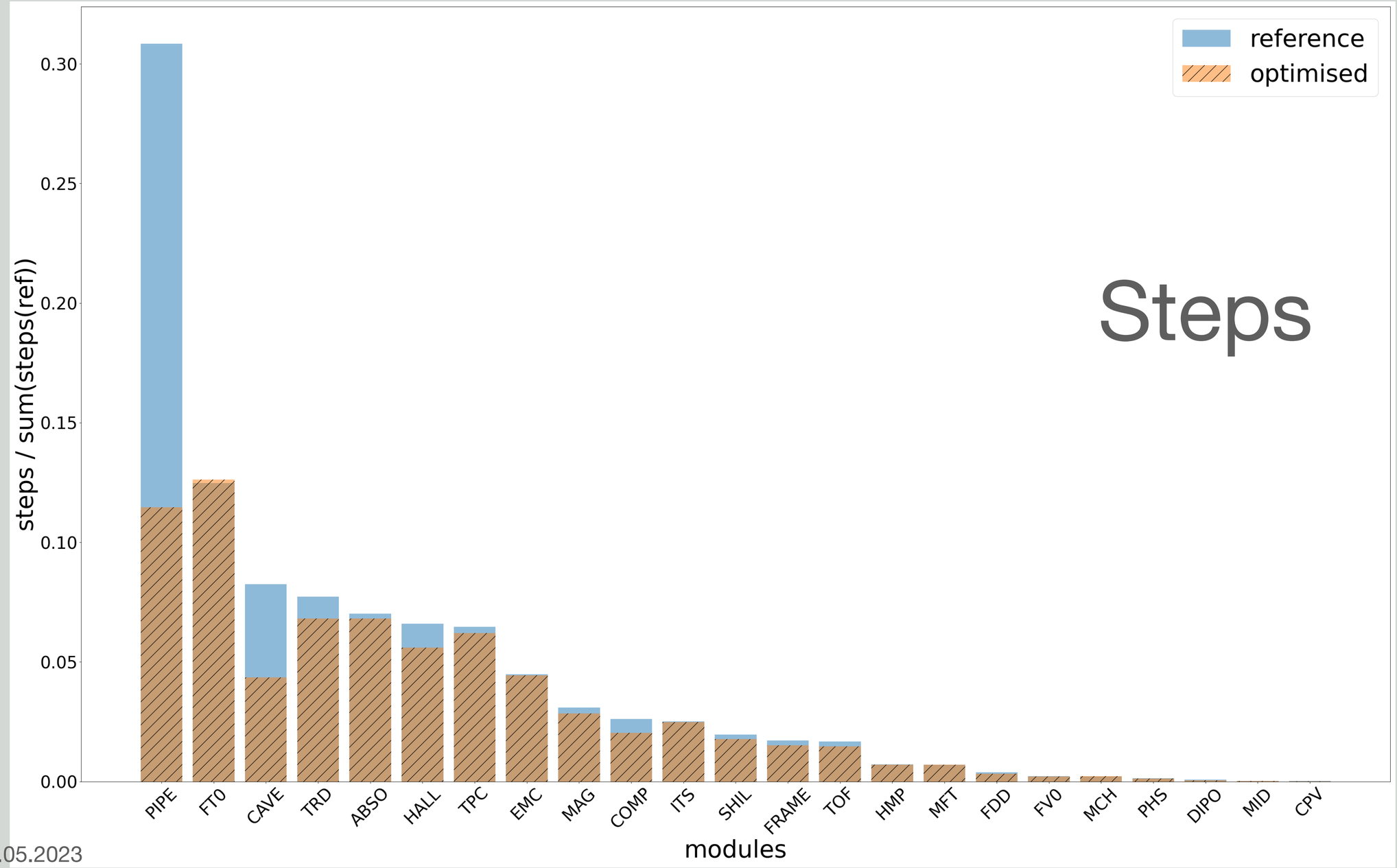
Optimised values of electromagnetic cut parameters



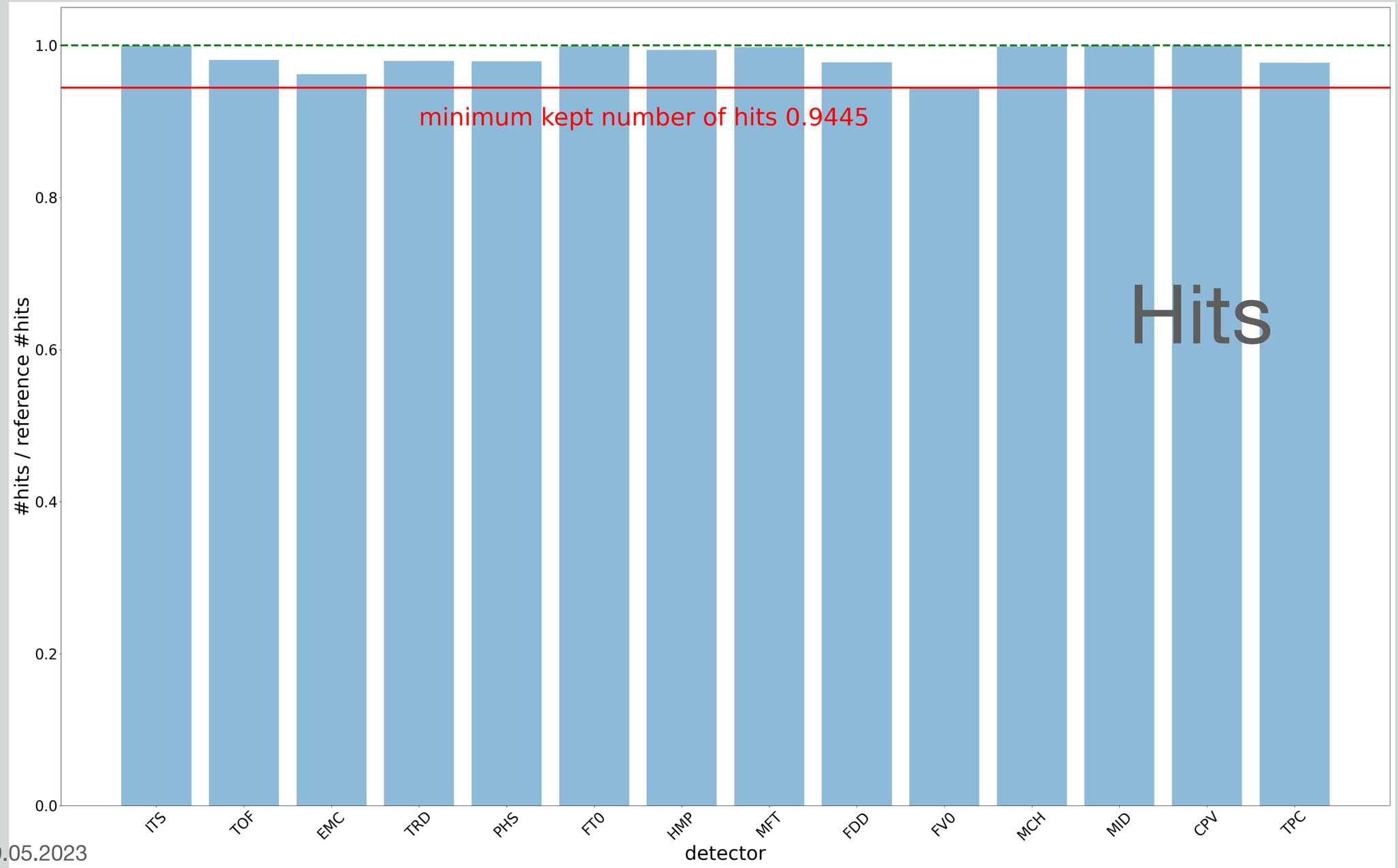
Many parameters changed by 1-3 orders of magnitude.

In this case (electromagnetic), cutting on electrons(photons) has a strong impact on the abundance of photons(electrons).

Removed more than 20% of all steps…



…while keeping almost all hits



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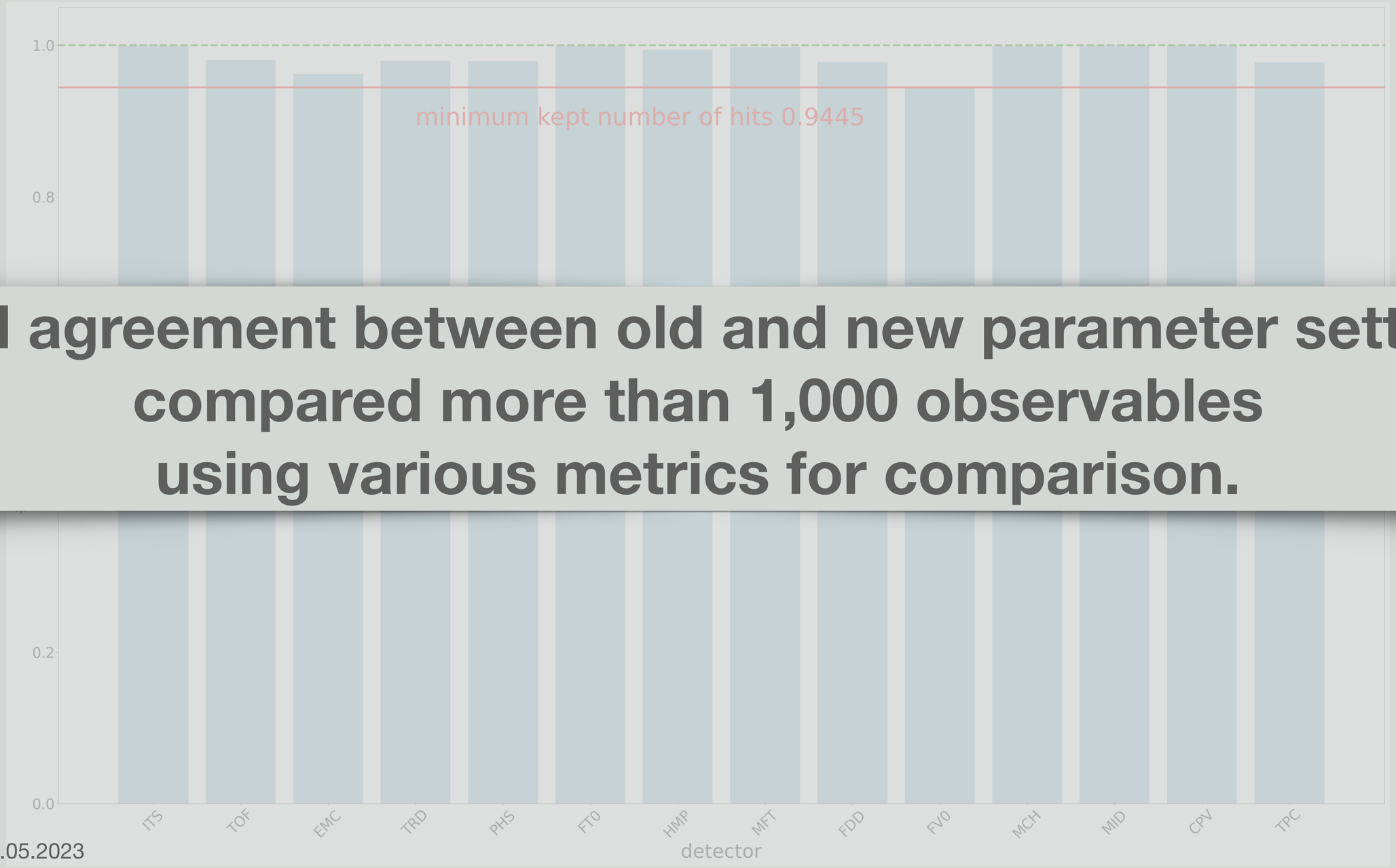


Good agreement between old and new parameter settings, compared more than 1,000 observables using various metrics for comparison.

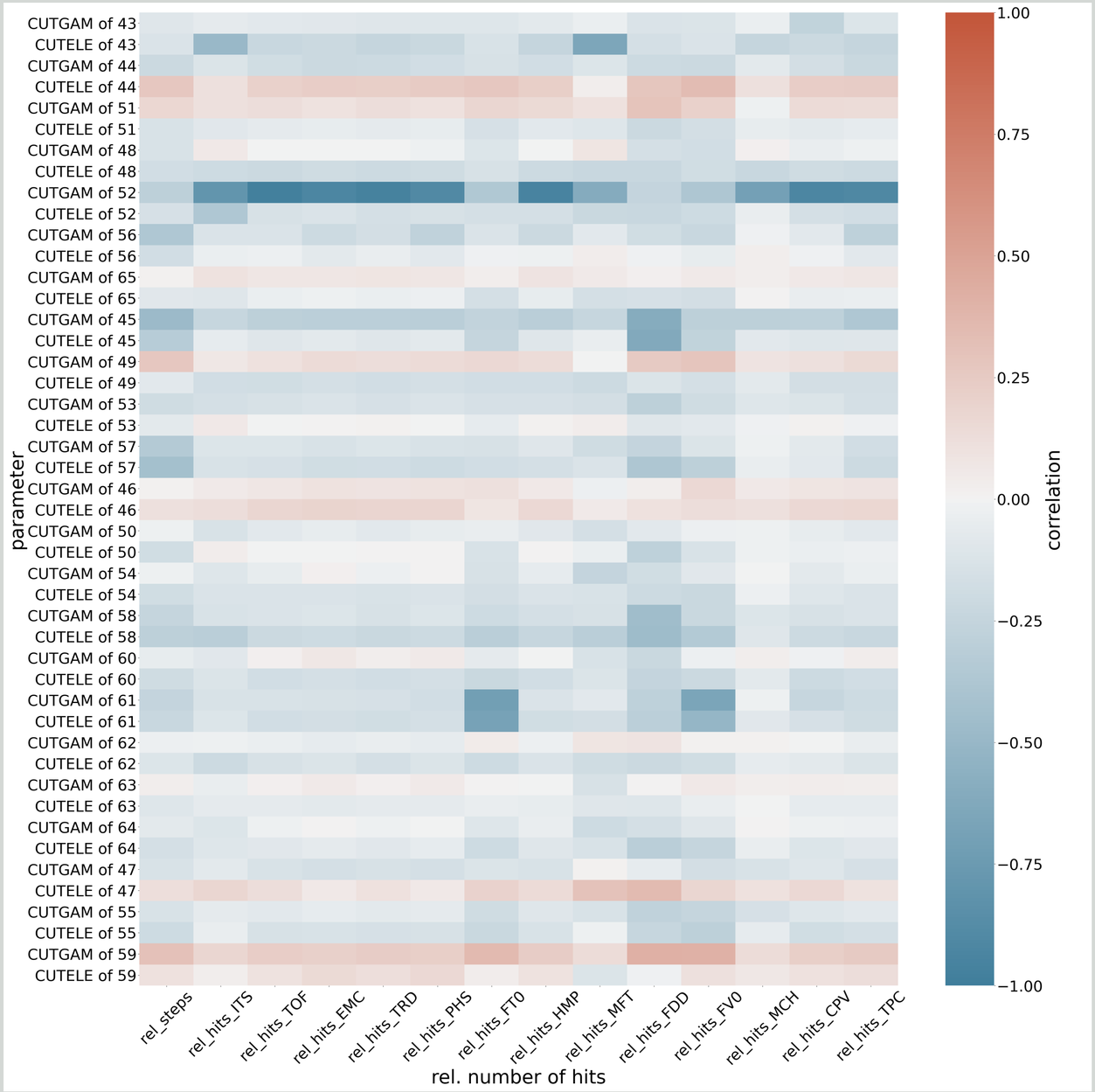
Bon Appetit!

- Gain 20% speed-up of full-simulation (only beam pipe).
- We will target other geometry or phase-space related parameters in such optimisations.
  - Now, the focus lies on further passive modules.
  - After that, we target additional parameters.
- Not only applicable to transport simulation but also to other parts of the simulation chain.
  [Digitisation, reconstruction, tracking…]
- Our studies teach us more about our detector as well as our simulation algorithms.
  [Provide valuable insight towards potential fast-simulation approaches.]

Thank you very much,
enjoy dinner,
and have a great conference!

BACKUP

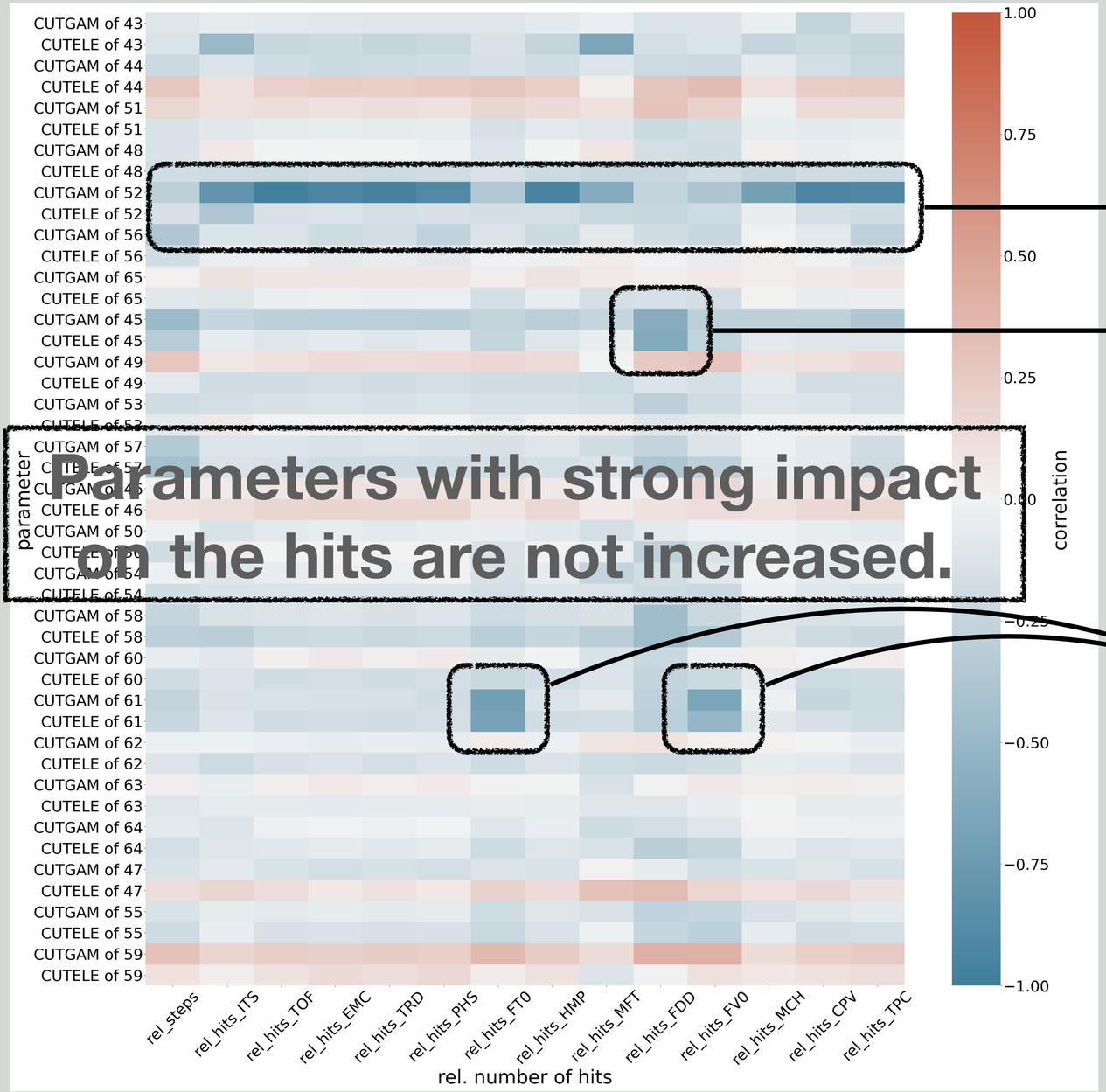
Parameters and hits go well together



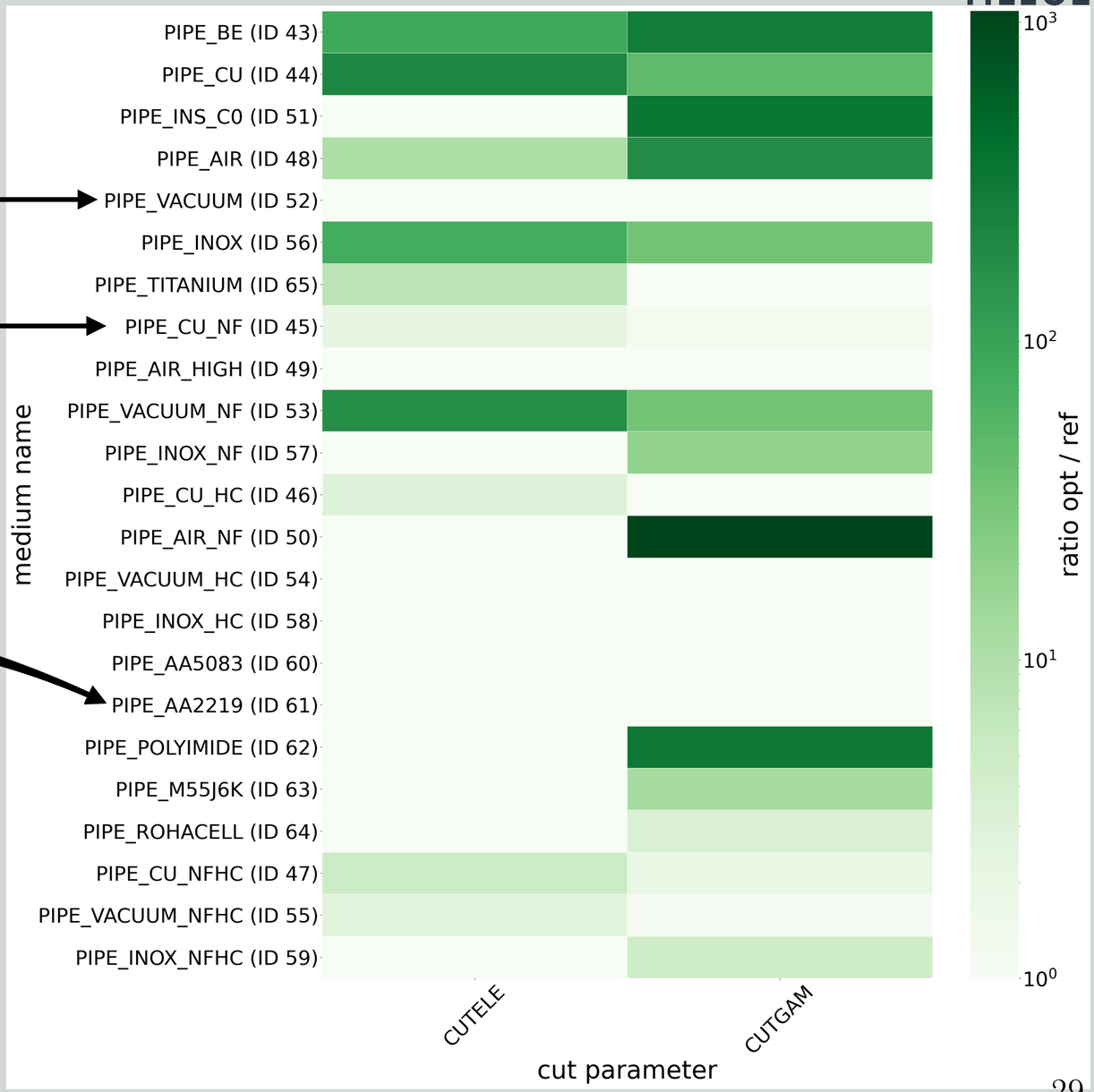
Correlation of number of kept hits with chosen cut value across all optimisation trials.

- A negative correlation basically means higher/lower cut ~ less/more hits.
- Intuitively, a positive correlation physically does not make sense. However, we are only looking at a “first order” relation between the hits and cuts. The choice of cut values is more complex!

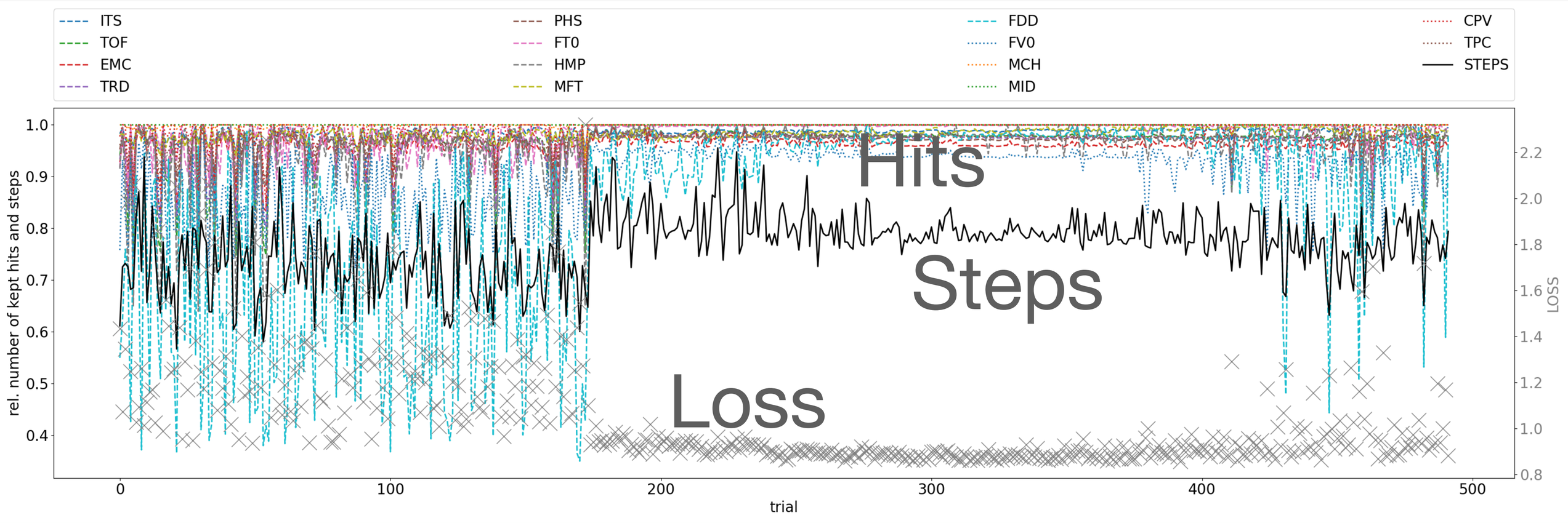
Parameters and hits go really well together



Parameters with strong impact on the hits are not increased.



Evolution of steps and hits during optimisation



“Warm-up” (drawing random parameters) for 150 trials. | **Optimising** | **Exhausted**