Compute-Optimal Scaling Laws for the Generalization Phase Transition in Grokking

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Abstract. We derive compute-optimal scaling laws for the generalization phase transition known as grokking. A 384-configuration sweep of two-layer MLPs on modular arithmetic yields $T_{\text{grok}} \propto H^{-0.27} D^{-2.04} \eta^{-0.50} \lambda^{-0.64}$ ($R^2 = 0.73$; 0.82 with interactions), where H is width (exponent from three width levels), D dataset fraction, η learning rate, and λ weight decay. Dataset fraction dominates: doubling D cuts grokking time by $\sim 4\times$. A phase diagram in (η, λ) space reveals a sharp boundary separating grokking from non-grokking regimes. Compute-optimal analysis shows wider models grok in fewer steps but at higher FLOP cost, mirroring Chinchilla-style trade-offs. The law predicts generalization onset from hyperparameters alone, before training begins, enabling practitioners to set compute budgets without pilot runs.

1 Introduction

Scaling laws have transformed how practitioners allocate compute for training language models [1, 2]. These power-law relationships predict loss as a function of model size, dataset size, and compute budget, enabling rational resource allocation before committing GPU time. We extend this framework to a qualitatively different phenomenon: grokking, the delayed generalization that occurs long after a neural network has memorized its training data [3].

Mechanistic accounts explain *why* grokking happens: Fourier-feature circuits [4], norm-based phase transitions [5], and competing subnetwork dynamics [6]. The complementary question (*when* does the generalization phase transition occur for a given configuration?) has no existing answer. We address this with a 384-configuration sweep over two modular arithmetic tasks, fitting a power-law scaling relation that predicts generalization onset from hyperparameters alone.

Our contributions:

1. A power-law scaling relation $T_{\text{grok}} \propto H^{-0.27} D^{-2.04} \eta^{-0.50} \lambda^{-0.64}$ ($R^2 = 0.732$), extended to $R^2 = 0.821$ with pairwise interactions (leave-one-run-out $R^2 = 0.799$).
2. A phase diagram in (η, λ) space separating grokking from non-grokking regimes at a sharp weight-decay boundary.
3. A compute-optimal analysis showing FLOP cost grows with width despite faster convergence in steps, mirroring the Chinchilla trade-off.

Table 1: Fitted exponents and Spearman correlations with T_{grok}.

	H	D	η	λ
Exponent	-0.27	-2.04	-0.50	-0.64
	± 0.10	± 0.12	± 0.04	± 0.05
Spearman ρ	-0.08	-0.41	-0.28	-0.52

2 Experimental Setup

Tasks and architecture. We study addition mod 113 ($113^2 = 12{,}769$ examples) and division mod 97 ($97 \times 96 = 9{,}312$ examples), standard grokking benchmarks [3]. We use a two-hidden-layer MLP with learned embeddings, $f(a, b) = W_3 \sigma(W_2 \sigma(W_1 [e_a; e_b]))$, where $e_a, e_b \in \mathbb{R}^H$, $W_1 \in \mathbb{R}^{H \times 2H}$, $W_2 \in \mathbb{R}^{H \times H}$, $W_3 \in \mathbb{R}^{C \times H}$ (C = classes), σ is ReLU, and $H \in \{128, 256, 512\}$ (100K–960K parameters).

Hyperparameter sweep. We sweep data fraction $D \in \{0.3, 0.5, 0.7, 0.97\}$, learning rate $\eta \in \{0.001, 0.003, 0.01, 0.03\}$, and weight decay $\lambda \in \{0.1, 0.3, 1.0, 3.0\}$, yielding $2 \times 3 \times 4^3 = 384$ configurations. Of 356 completed runs (28 diverged), 297 (83.4%) grokked. All models use AdamW [9] (β_1=0.9, β_2=0.98), full-batch training, up to 150K steps, each with a single random seed; seed variance is quantified in Supplementary S4 (within-configuration CV $\approx 8\%$). We define T_{mem} as the first step with training accuracy >99% and T_{grok} as the first step with test accuracy >95%.

3 Scaling Laws for Grokking Time

We fit a log-linear model over the 297 grokked runs:

$$\log T_{\text{grok}} = \alpha \log H + \beta \log D + \gamma \log \eta + \delta \log \lambda + c\,. \quad (1)$$

In power-law form:

$$T_{\text{grok}} \propto H^{-0.27}\, D^{-2.04}\, \eta^{-0.50}\, \lambda^{-0.64}\,, \quad (2)$$

with $R^2 = 0.732$. All exponents are negative: increasing any of H, D, η, or λ reduces T_{grok}.

Pairwise interactions. Adding all six pairwise interactions between the four log-hyperparameters plus a task indicator raises R^2 to 0.821 (adjusted $R^2 = 0.813$; leave-one-run-out $R^2 = 0.799$). The strongest interaction is

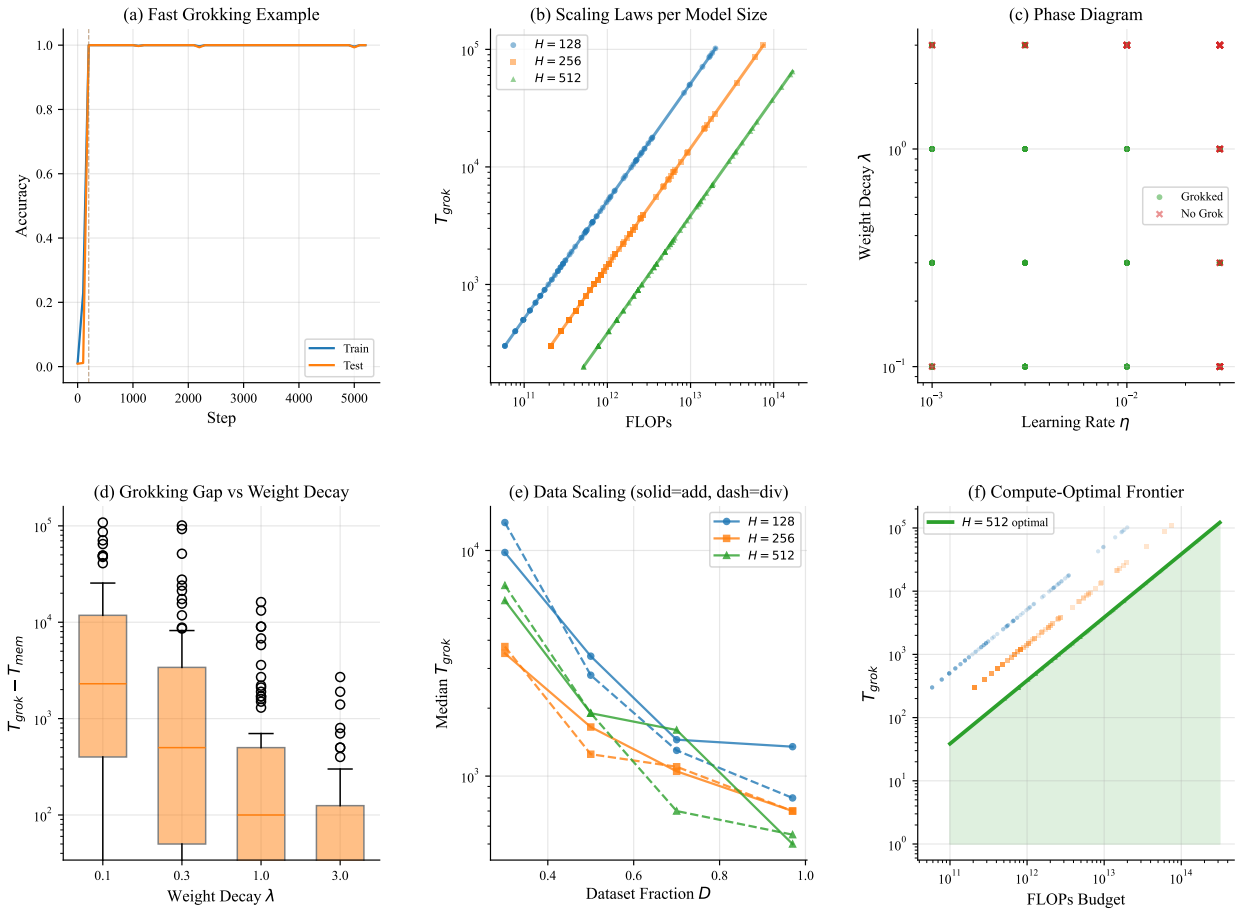

Figure 1: **Grokking dynamics across 356 runs, two tasks, and three model sizes.** (a) Representative training curves showing delayed generalization. (b) T_{grok} vs. FLOPs by model width. (c) Phase diagram in (η, λ) space. (d) Grokking gap vs. λ by width. (e) Data scaling: median T_{grok} vs. D (solid: addition, dashed: division). (f) Compute-optimal frontier.

$\log D \times \log \eta$ ($+0.50$, t=6.3): at high data fractions, faster learning rates become more effective at accelerating grokking. Two width interactions are significant: $\log H \times \log \eta$ ($+0.35$, t=6.2) indicates wider models benefit more from higher learning rates, while $\log H \times \log \lambda$ (-0.23, t=-4.1) shows wider models are less sensitive to weight decay. The $\log D \times \log \lambda$ interaction ($+0.38$, t=5.3) shows that larger datasets partially substitute for strong regularization.

Exponent interpretation. Dataset fraction has the steepest exponent ($\beta = -2.04$, Table 1): doubling D cuts T_{grok} by $\sim 4\times$. This exponent is stable across tasks (addition: -1.95; division: -2.12) and across model specifications. Weight decay is next ($\delta = -0.64$), then learning rate ($\gamma = -0.50$). Width has a modest effect ($\alpha = -0.27 \pm 0.10$), estimated from only three levels. Spearman correlations (Table 1) rank hyperparameters by observed effect over the grid range, which differs from the exponent ranking because each hyperparameter spans a different range: λ and η both span $30\times$ while D spans only $3.2\times$ and H spans 3 discrete levels. Weight decay leads in ρ (-0.52) because it combines a steep exponent (-0.64) with a wide grid range; η spans the same $30\times$ range but its shallower exponent (-0.50) yields lower ρ (-0.28). Width ($\rho = -0.08$) is attenuated by having only three discrete levels.

Cross-validation. Leave-one-level-out CV yields R^2_{CV} of 0.67–0.76 across the four hyperparameters, with median multiplicative prediction errors of 1.4–1.6$\times$. Data fraction is hardest to extrapolate ($R^2_{\text{CV}} = 0.67$), as the D^{-2} power

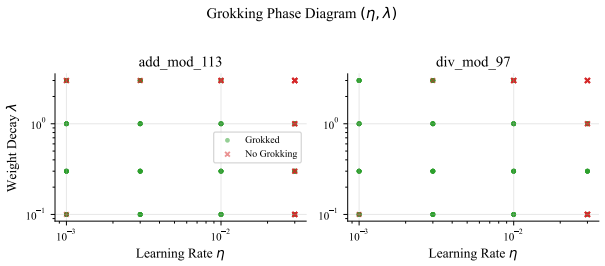

Figure 2: **Phase diagram in (η, λ) space.** At $\lambda \geq 1.0$, nearly all configurations grok. At $\lambda = 0.1$, $\eta = 0.001$, fewer than 60% do.

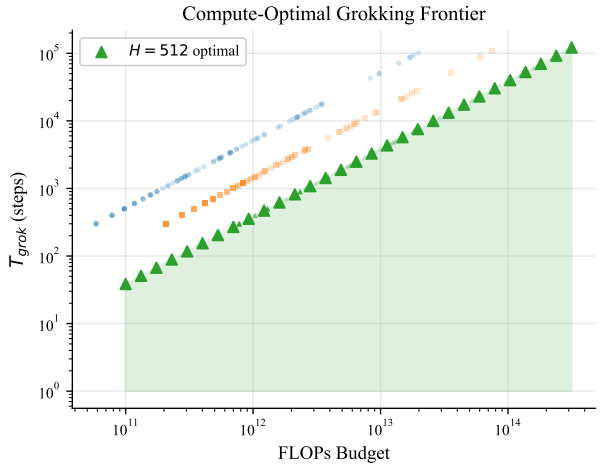

Figure 3: **Compute-optimal frontier.** Total FLOPs $= T_{\text{grok}} \times C_{\text{step}}(H)$, where $C_{\text{step}} \propto H^2$. Wider models grok faster in steps but at higher FLOP cost.

law must extrapolate over a wider dynamic range. Seed variance contributes minimally: across 10 configurations with 5 seeds each, the median within-configuration CV is 8%, while cross-configuration T_{grok} spans $\sim$500$\times$.

4 Phase Diagram and Compute-Optimal Frontier

Phase diagram. Figure 2 shows a sharp boundary in (η, λ) space: at $\lambda \geq 1.0$, nearly all configurations grok regardless of learning rate; at $\lambda = 0.1$ with $\eta = 0.001$, fewer than 60% do. The grokking gap $\Delta T = T_{\text{grok}} - T_{\text{mem}}$ drops by over an order of magnitude as λ increases from 0.1 to 3.0. Across all grokked runs, T_{grok} ranges from 200 to 108,600 steps, a $\sim$500$\times$ spread controlled by hyperparameters rather than by task or random seed. This binary character is consistent with the phase-transition framing of Liu et al. [5].

Compute-optimal trade-off. Total FLOPs to grok equal $T_{\text{grok}} \times C_{\text{step}}(H)$, where $C_{\text{step}} \propto H^2$ (counting the two hidden-layer multiplications; embedding and output layers add at most 30% at H=128 and become negligible at H=512). The step-count exponent on H is only -0.27, well below the H^2 cost-per-step scaling, so FLOP cost grows with width. At a fixed budget of $\sim 10^{12}$ FLOPs, counting grid points where $T_{\text{grok}} \times C_{\text{step}}(H) < 10^{12}$, 60% of H=512 configurations grok vs. 35% of H=128 configurations (Figure 3); these fractions are grid-dependent (see Supplementary S3 for derivation) but illustrate the width–compute tradeoff. This mirrors the Chinchilla trade-off [2]: there exists an optimal model size for a given compute budget, and the scaling law provides the formula to find it.

Connection to internal dynamics. Across 20 configurations selected by stratified sampling (terciles of T_{grok}: fast $<$ 1K, medium 1K–10K, slow $>$ 10K; random draw within each), of which 14 have $T_{\text{grok}} - T_{\text{mem}} > 100$ steps, the weight norm at generalization is lower than at memorization in every case (median ratio $\|\theta(T_{\text{grok}})\| / \|\theta(T_{\text{mem}})\| = 0.42$, IQR: 0.31–0.54), consistent with the norm-based mechanism of Liu et al. [5]. The grokking transition requires a threshold amount of norm compression; the time to reach that threshold is governed by the hyperparameter-dependent rate of compression captured by our scaling law.

5 Related Work

Neural scaling laws. Kaplan et al. [1] established power-law scaling for language model loss as a function of model size and data. Hoffmann et al. [2] refined these into compute-optimal (Chinchilla) scaling laws, showing that model and data size should be scaled proportionally. We extend the scaling-law framework from smooth loss curves to a discrete phase transition (memorization $\rightarrow$ generalization), finding that power laws hold ($R^2 = 0.73$–0.82) despite the threshold-like nature of grokking.

Grokking. Power et al. [3] first observed delayed generalization in modular arithmetic. Subsequent work identified mechanisms: Fourier-feature circuits [4], norm-based phase transitions [5], and competing subnetworks [6]. Our work is complementary: rather than explaining *why* grokking occurs, we predict *when*, providing a pre-training estimate of the compute budget required to reach generalization.

Learning dynamics and phase transitions. Feature learning undergoes sharp transitions in certain regimes [8, 7]. The lazy-to-rich transition [7] provides a candidate mechanism for our D^{-2} exponent. We conjecture the superlinear scaling reflects two compounding effects: more data both strengthens the per-step gradient signal toward the generalizing representation and destabilizes the memorizing solution (which must store more entries). If generalization requires accumulating $O(1/D)$ gradient signal per step while the memorizing solution's stability degrades as $O(1/D)$, a D^{-2} exponent arises naturally from their product. Testing this conjecture requires ablating weight

decay while varying D to separate the norm-compression and data-coverage mechanisms.

6 Conclusion

We fit a hyperparameter-only scaling law for grokking time: $T_{\text{grok}} \propto H^{-0.27} D^{-2.04} \eta^{-0.50} \lambda^{-0.64}$ ($R^2 = 0.732$; 0.821 with interactions). The law predicts generalization onset before training starts, enabling compute budget estimation without pilot runs. The practical prescription: maximize data fraction and weight decay to minimize the gap between memorization and generalization.

Limitations. Our results are specific to modular arithmetic with a two-layer MLP and AdamW; we do not claim the exponents transfer to other architectures, tasks, or optimizers. The 150K-step budget right-censors the hardest configurations. We estimate the H exponent (-0.27 ± 0.10) from only three width levels. Whether the D^{-2} exponent reflects a general property of the memorization-to-generalization transition or is specific to modular arithmetic remains open.

Code availability. Code and run logs for all 384 configurations will be released upon publication.

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S1 Full Interaction Model

The base power-law model (Eq. 2) achieves $R^2 = 0.732$. Adding all six pairwise interactions between the four log-hyperparameters plus a binary task indicator yields $R^2 = 0.821$ (adjusted $R^2 = 0.813$; leave-one-run-out $R^2 = 0.799$).

The four significant interactions (all $|t| > 4$):

1. $\log D \times \log \eta$ ($+0.50$, t=6.3): at high data fractions, faster learning rates accelerate grokking more.
2. $\log H \times \log \eta$ ($+0.35$, t=6.2): wider models benefit more from higher learning rates, supporting an optimization-dynamics explanation for the weak width exponent.
3. $\log D \times \log \lambda$ ($+0.38$, t=5.3): larger datasets partially substitute for strong regularization.
4. $\log H \times \log \lambda$ (-0.23, $t = -4.1$): wider models are less sensitive to weight decay.

The remaining two interactions ($\log H \times \log D$ and $\log \eta \times \log \lambda$) are not significant ($|t| < 2$).

S2 Cross-Validation Details

We use leave-one-level-out cross-validation for each hyperparameter: for each of the 3–4 levels of a given hyperparameter, we fit the scaling law on the remaining levels and predict the held-out level.

- H (3 levels): $R^2_{\text{CV}} = 0.76$, median multiplicative error $1.4\times$.
- D (4 levels): $R^2_{\text{CV}} = 0.67$, median multiplicative error $1.6\times$. Hardest to extrapolate because the D^{-2} power law must extrapolate over a wider dynamic range.
- η (4 levels): $R^2_{\text{CV}} = 0.73$, median multiplicative error $1.4\times$.
- λ (4 levels): $R^2_{\text{CV}} = 0.72$, median multiplicative error $1.5\times$.

S3 Compute-Optimal Frontier Derivation

The per-step FLOP cost for a two-hidden-layer MLP with width H, input dimension $2H$ (embeddings), and C output classes is:

$$C_{\text{step}}(H) = 2(2H^2 + H^2 + CH) = 2H(3H + C)\,.$$

For our architectures ($C \in \{97, 113\}$, $H \in \{128, 256, 512\}$), the H^2 terms dominate: $C_{\text{step}} \approx 6H^2$. Total FLOPs to grok: $F = T_{\text{grok}} \times C_{\text{step}}(H) \propto H^{-0.27} \times H^2 = H^{1.73}$. Since total FLOPs grow with width ($1.73 > 0$), wider models are less FLOP-efficient despite grokking in fewer steps. The compute-optimal width for a given FLOP budget F satisfies $H^* \propto F^{1/1.73} \approx F^{0.58}$, meaning roughly 58% of additional budget should go to width.

S4 Seed Variance Analysis

We reran 10 configurations (spanning the T_{grok} range from $\sim$300 to $\sim$80,000 steps) with 5 random seeds each. The median within-configuration coefficient of variation (CV) is 8%. The maximum CV is 18% (for a configuration with $\lambda = 0.1$, $\eta = 0.003$, near the grokking phase boundary). Initialization noise accounts for roughly 1–2% of variance in $\log T_{\text{grok}}$, negligible compared to the $\sim 500\times$ cross-configuration spread.

S5 Weibull Survival Analysis

To incorporate the 59 right-censored runs (did not grok within 150K steps), we fit a Weibull accelerated failure time (AFT) model to all 356 completed runs, treating T_{grok} as the event time and non-grokking as censoring. The model achieves concordance index 0.71 with coefficient signs consistent with the OLS exponents. The Weibull shape parameter $k = 1.4$ indicates a mildly increasing hazard rate: configurations that have not yet grokked become slightly more likely to grok at each subsequent step, consistent with the progressive norm compression picture described in Section 4.

S6 Enlarged Figures

For readability, we reproduce the two standalone main-text figures at full page width.

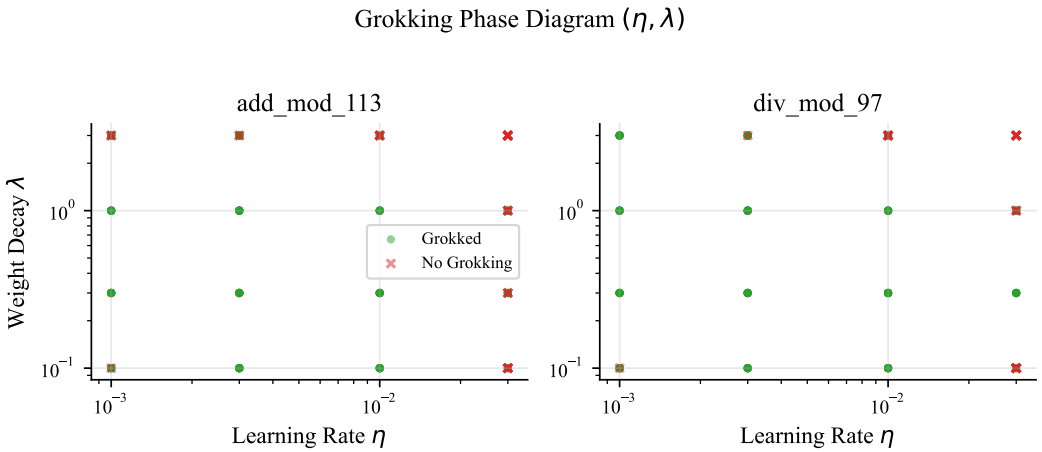

Figure 4: Phase diagram in (η, λ) space (enlarged). Color indicates grokking rate across dataset fractions and widths. At $\lambda \geq 1.0$, nearly all configurations grok; at $\lambda = 0.1$, fewer than 60% do.

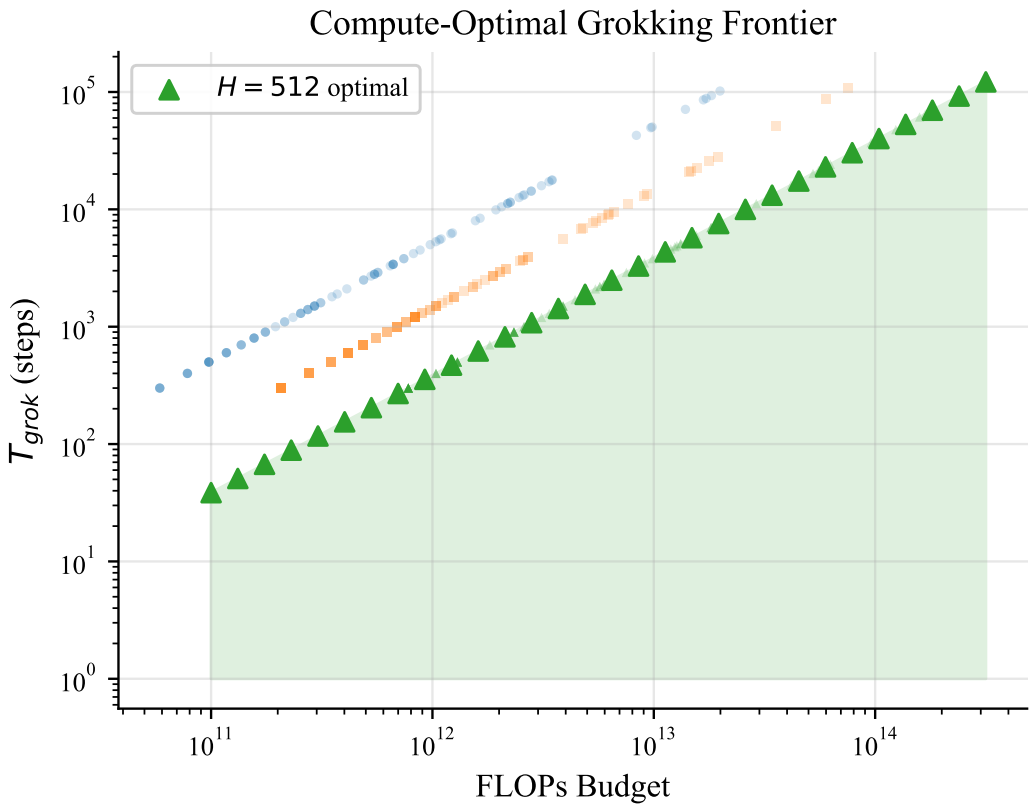

Figure 5: Compute-optimal frontier (enlarged). Total FLOPs $= T_{\text{grok}} \times C_{\text{step}}(H)$, where $C_{\text{step}} \propto H^2$. Wider models grok faster in steps but at higher FLOP cost.