

# cuML-DSA: Optimized Signing Procedure and Server-Oriented GPU Design for ML-DSA

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**Abstract**—The threat posed by quantum computing has precipitated an urgent need for post-quantum cryptography. Recently, the post-quantum digital signature draft FIPS 204 has been published, delineating the details of the ML-DSA, which is derived from the CRYSTALS-Dilithium. Despite these advancements, server environments, especially those equipped with GPU devices necessitating high-throughput signing, remain entrenched in classical schemes. A conspicuous void exists in the realm of GPU implementation or server-specific designs for ML-DSA.

In this paper, we propose the first server-oriented GPU design tailored for the ML-DSA signing procedure in high-throughput servers. We introduce several innovative theoretical optimizations to bolster performance, including depth-prior sparse ternary polynomial multiplication, the branch elimination method, and the rejection-prioritized checking order. Furthermore, exploiting server-oriented features, we propose a comprehensive GPU hardware design, augmented by a suite of GPU implementation optimizations to further amplify performance. Additionally, we present variants for sampling sparse polynomials, thereby streamlining our design. The deployment of our implementation on both server-grade and commercial GPUs demonstrates significant speedups, ranging from  $284.9\times$  to  $485.3\times$  against the CPU baseline, and an improvement of up to 60.9% compared to related work, affirming the effectiveness and efficiency of the proposed GPU architecture for ML-DSA signing procedure.

**Index Terms**—post-quantum cryptography, digital signature, ML-DSA, sparse polynomial multiplication, GPU acceleration.

## I. INTRODUCTION

**D**IGITAL signatures, serving as the bedrock for data integrity and authentication, have always been indispensable in the realm of data security. The essence lies in detecting unauthorized alterations to data and validating the identity of the signatory. However, the strides in quantum computing technology threaten the foundation of existing digital signature schemes primarily based on integer factorization and discrete logarithms [1]. Such schemes, while robust against classical computing attacks, crumble before quantum computers.

Recognizing the impending challenge, there has been an international endeavor to identify and standardize cryptographic algorithms resistant to quantum attacks. Spearheading this movement, the National Institute of Standards and Technology (NIST) initiated an extensive public vetting process in search of quantum-resistant public-key cryptographic algorithms [2]. This rigorous initiative saw a deluge of proposals, reflecting the global urgency and effort in thwarting quantum threats.

After three rounds, NIST select one key encapsulation mechanism (KEM) and three digital signature algorithms for standardization in commerce, where the CRYSTALS-Dilithium emerged as the primary choice [3]. The recent unveiling of the draft standard FIPS 204 [4] epitomizes this endeavor, detailing the ML-DSA (Module Lattice Digital Signature Algorithm) – a derivative of the Dilithium [5], [6]. This standard promises strong unforgeability and is envisioned to provide long-term security in the impending quantum era.

In the commercial arena, throughput is not just desirable, but indispensable. Contemporary businesses grapple with an immense volume of online transactions, each utilizing digital signatures to guarantee message integrity and authenticity. This necessitates the implementation of high-throughput and real-time cryptographic solutions. Servers, being the backbone of such transactions, need designs emphasizing throughput. One of the key allies in this challenge is the GPU. With its inherent parallelism, GPUs offer concurrent processing capabilities, making them prime candidates for accelerating server-grade tasks. Recent literature showcases several optimizations of Dilithium, targeting diverse hardware like ASICs and FPGAs [7]–[9], and software platforms ranging from high-performance processors [10]–[13] to embedded devices [14], [15]. Moreover, while GPU implementations of post-quantum KEMs abound [16]–[21], there is a conspicuous dearth of GPU implementations for post-quantum digital signature schemes [11], [12], [22], and high-throughput designs remain largely in classical schemes. To date, there exists no GPU design of the ML-DSA and for Dilithium, only studies [11], [12] have been reported.

**Contributions.** In this work, we introduce several theoretical optimizations as well as the first server-centric GPU design for the ML-DSA signing procedure. Our aim is to enhance both signing performance and throughput. A summary of our contributions is as follows:

- *Optimization of the Rejection Process.* Utilizing the sparse ternary polynomial multiplication technique, we introduce an enhanced depth-prior version that facilitates earlier rejection, and we leverage both vertical and horizontal parallelism to bolster parallelism. Then, we present a method to eradicate branching, promoting constant-time execution which is more amenable to parallel operations. Additionally, we recommend a rejection-prioritized norm checking sequence for the initial three checks, allowing for more prompt identification of invalid signatures.
- *Server-Oriented Design.* We delve into the possible accelerations that a server-centric design might offer and put forward a comprehensive hardware architecture for the

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ML-DSA signing process. Then, we introduce an optimized GPU acceleration engine, accompanied by several implementation enhancements. These include integration with early evaluation, refined memory access patterns, and the caching of key component, resulting a reduction in IO latency and an uptick in overall performance.

- **Performance Analysis.** We execute our implementation on both server-grade and commercial GPUs, assessing both batching and streaming methods. Compared to the CPU baseline, we achieve performance gains of  $271.6\times$  to  $333.9\times$  on the A100 and  $348.1\times$  to  $485.3\times$  on the 4090 GPU across the three parameter sets. In comparison to the AVX2 optimized implementation, our implementation is faster by factors ranging from  $60.3\times$  to  $75.7\times$  on the A100 and  $73.6\times$  to  $110.0\times$  on the 4090 GPU. Furthermore, we record improvements of up to  $60.9\%$  against recent GPU-based work on identical platforms.

## II. PRELIMINARIES

### A. Notation

Let  $n$  be a power of two and  $q$  a prime where  $q \equiv 1 \pmod{2n}$ . Define  $\mathbb{Z}$  as the integer set, and  $R = \mathbb{Z}[X]/(X^n + 1)$  as the  $2n$ -th cyclotomic ring. Additionally,  $\mathbb{Z}_q$  is defined as  $\mathbb{Z}/q\mathbb{Z}$ , while  $R_q$  is given by  $R/qR \cong \mathbb{Z}_q[X]/(X^n + 1)$ . We use integer intervals, e.g.,  $[0, n] = \{0, 1, \dots, n\}$ .

Elements in  $R$  (or  $R_q$ ) are represented as polynomials, typically denoted by bold, italic lowercase letters (e.g.,  $\mathbf{f}$ ). Vectors are indicated using bold, upright lowercase letters (e.g.,  $\mathbf{x}$ ). Each polynomial  $\mathbf{f} \in R$  or  $R_q$  is expressed as  $\mathbf{f} = \sum_{i=0}^{n-1} f_i X^i$ , where  $f_i \in \mathbb{Z}$  or  $\mathbb{Z}_q$  for  $i \in [0, n]$ . Matrices over  $R$  or  $R_q$  use uppercase boldface letters (e.g.,  $\mathbf{M}$ ). For a polynomial  $\mathbf{f} \in R$ , its  $\ell_\infty$ -norm is given by  $\|\mathbf{f}\|_\infty = \max\{|f_i|\}$ . Similarly, for a vector  $\mathbf{x} = (x_0, x_1, \dots, x_{n-1}) \in R^n$ , its  $\ell_\infty$ -norm is defined as  $\|\mathbf{x}\|_\infty = \max\{|x_i|\}$ .

### B. Polynomial Multiplication

Given polynomials  $\mathbf{a} = \sum_{i=0}^{n-1} a_i X^i$ ,  $\mathbf{c} = \sum_{i=0}^{n-1} c_i X^i \in R_q$ , their multiplication over  $R_q$  yields  $\mathbf{b} = \sum_{i=0}^{n-1} b_i X^i$ . We discuss two common methods to compute this result.

**Number-Theoretic Transform (NTT).** The NTT is an efficient strategy for polynomial multiplications in  $R_q$ . Let  $\zeta$  be the primitive  $2n$ -th root of unity. This method applies forward NTT to  $\mathbf{a}$  and  $\mathbf{c}$ , performs point-wise multiplication in the NTT domain, and applies inverse NTT to the result. The process is formulated as:

$$\begin{aligned} \hat{\mathbf{a}} &= \sum_{j=0}^{n-1} \hat{a}_j X^j := \text{NTT}(\mathbf{a}), \hat{a}_j = \sum_{i=0}^{n-1} a_i \zeta^{(2i+1)j} \pmod{q} \\ \mathbf{a} &= \sum_{i=0}^{n-1} a_i X^i := \text{INTT}(\hat{\mathbf{a}}), a_i = \frac{1}{n} \sum_{j=0}^{n-1} \hat{a}_j \zeta^{-(2i+1)j} \pmod{q} \end{aligned}$$

Then, performing  $\mathbf{b} = \mathbf{a} \cdot \mathbf{c} = \text{INTT}(\text{NTT}(\mathbf{a}) \cdot \text{NTT}(\mathbf{c}))$  yields the result. This reduces computational complexity from  $\mathcal{O}(n^2)$  to  $\mathcal{O}(n \log n)$ , thus improving the performance.

**Sparse Ternary Polynomial Multiplication (STPM).** For polynomial  $\mathbf{b} = \mathbf{a} \cdot \mathbf{c} = \sum_{k=0}^{n-1} b_k X^k$ , the schoolbook method computes each coefficient of  $\mathbf{b}$  as:

### Algorithm 1 Sparse ternary polynomial multiplication

**Input:**  $\mathbf{c} = \sum_{i=0}^{n-1} c_i \cdot x^i \in B_\tau$ ,  $\mathbf{a} = \sum_{i=0}^{n-1} a_i \cdot x^i \in R_q$   
**Output:**  $\mathbf{u} = \mathbf{c} \cdot \mathbf{a} \in R_q$   
1: **for**  $i \in [0, n)$  **do**  
2:    $w_i := 0$ ,  $v_i := a_i$ ,  $v_{i-n} := -a_i$   
3: **for**  $i \in [0, n)$  **do**  
4:   **if**  $c_i = 1$  **then**  
5:     **for**  $j \in [0, n)$  **do**  
6:        $w_j := w_j + v_{j-i}$   
7:   **if**  $c_i = -1$  **then**  
8:     **for**  $j \in [0, n)$  **do**  
9:        $w_j := w_j - v_{j-i}$   
10: **for**  $i \in [0, n)$  **do**  
11:    $u_i := w_i \pmod{q}$   
12: **return**  $\mathbf{u} = \sum_{i=0}^{n-1} u_i \cdot x^i$

### Algorithm 2 ML-DSA.Sign

**Input:**  $sk = (\rho, K, tr, \mathbf{s}_1, \mathbf{s}_2, \mathbf{t}_0)$ ,  $M \in \{0, 1\}^*$   
•  $\rho, K, tr \in \{0, 1\}^{256}$   
•  $\mathbf{s}_1 := [\mathbf{s}_1^{(0)}, \dots, \mathbf{s}_1^{(\ell-1)}] \in R_q^\ell$ ,  $\mathbf{s}_2 := [\mathbf{s}_2^{(0)}, \dots, \mathbf{s}_2^{(k-1)}] \in R_q^k$   
•  $\mathbf{t}_0 := [\mathbf{t}_0^{(0)}, \dots, \mathbf{t}_0^{(k-1)}] \in R_q^k$   
**Output:**  $\sigma = (\tilde{c}, \mathbf{z}, \mathbf{h})$   
1:  $\mu \in \{0, 1\}^{512} := \mathcal{H}(tr \| M)$   
2:  $rnd := \{0\}^{256}$  ▷ Deterministic variant  
3:  $\rho' \in \{0, 1\}^{512} := \mathcal{H}(K \| rnd \| \mu)$   
4:  $\hat{\mathbf{A}} \in R_q^{k \times \ell} := \text{ExpandA}(\rho)$   
5:  $\kappa := 0$ ;  $(\mathbf{z}, \mathbf{h}) := \perp$   
6: **while**  $(\mathbf{z}, \mathbf{h}) = \perp$  **do**  
7:    $\mathbf{y} \in S_{\gamma_1}^\ell := \text{ExpandMask}(\rho', \kappa)$   
8:    $\mathbf{w} := \hat{\mathbf{A}} \cdot \mathbf{y}$   
9:    $\mathbf{w}_1 := \text{HighBits}_q(\mathbf{w}, 2\gamma_2)$   
10:    $\tilde{c} := (\tilde{c}_1, \tilde{c}_2) \in \{0, 1\}^{256} \times \{0, 1\}^{2\lambda-256} := \mathcal{H}(\mu \| \mathbf{w}_1)$   
11:    $\mathbf{c} \in B_\tau := \text{SampleInBall}(\tilde{c}_1)$   
12:    $\mathbf{z} := \mathbf{y} + \mathbf{c} \cdot \mathbf{s}_1$   
13:    $\mathbf{r}_0 := \text{LowBits}_q(\mathbf{w} - \mathbf{c} \cdot \mathbf{s}_2, 2\gamma_2)$   
14:   **if**  $\|\mathbf{z}\|_\infty \geq \gamma_1 - \beta$  **or**  $\|\mathbf{r}_0\|_\infty \geq \gamma_2 - \beta$  **then**  
15:      $(\mathbf{z}, \mathbf{h}) := \perp$   
16:   **else**  
17:      $\mathbf{h} := \text{MakeHint}_q(-\mathbf{c} \cdot \mathbf{t}_0, \mathbf{w} - \mathbf{c} \cdot \mathbf{s}_2 + \mathbf{c} \cdot \mathbf{t}_0, 2\gamma_2)$   
18:     **if**  $\|\mathbf{c} \cdot \mathbf{t}_0\|_\infty \geq \gamma_2$  **or** number of 1's in  $\mathbf{h}$  exceeds  $\omega$  **then**  
19:        $(\mathbf{z}, \mathbf{h}) := \perp$   
20:    $\kappa := \kappa + \ell$

$$b_k = \sum_{i=0}^k a_i c_{k-i} - \sum_{i=k+1}^{n-1} a_i c_{k+n-i} \pmod{q}$$

The original computational complexity of this method is  $\mathcal{O}(n^2)$ . However, if  $\mathbf{c}$  is a sparse ternary polynomial with  $\tau$  non-zero coefficients ( $\pm 1$ ), we can optimize by evaluating  $\mathbf{c}$ 's coefficients and adding or subtracting  $\mathbf{a}$ 's coefficients. Algorithm 1 details this process. With  $\mathbf{c}$  having only  $\tau$  non-zero coefficients, multiplication complexity is reduced.

### C. ML-DSA and Parallel STPM

ML-DSA is a digital signature scheme proven strongly unforgeable in the QROM based on decisional Module-LWE and SelfTargetMSIS assumptions [4]. It emerges from the CRYSTALS-Dilithium, a proposal submitted to the NIST PQC standardization project. Algorithm 2 summarizes the signing procedure, with parameter sets in Table I. This function uses the secret key  $sk$  and message  $M$  as input and generates a valid signature  $\sigma := (\tilde{c}, \mathbf{z}, \mathbf{h})$  after several rounds of checks. The specifics of sub-procedures are available in [4]–[6].

TABLE I  
ML-DSA PARAMETER SETS.

Parameter Set	$n$	$q$	$d$	$\tau$	$\gamma_1$	$\gamma_2$	$(k, \ell)$	$\eta$	$\beta$	$\omega$	$\lambda$
ML-DSA-44	256	8380417	13	39	$2^{17}$	95232	(4,4)	2	78	80	128
ML-DSA-65	256	8380417	13	49	$2^{19}$	261888	(6,5)	4	196	55	192
ML-DSA-87	256	8380417	13	60	$2^{19}$	261888	(8,7)	2	120	75	256

**Algorithm 3** Parallel sparse ternary polynomial multiplication

**Input:**  $(\mathbf{c}, \mathbf{a})$ , where  $\mathbf{a} = [\mathbf{a}^{(0)}, \dots, \mathbf{a}^{(r-1)}]^T \in R_q^r$ , every  $\mathbf{a}^{(j)} = \sum_{i=0}^{n-1} a_i^{(j)} \cdot x^i \in R_q$ , and  $\mathbf{c} = \sum_{i=0}^{n-1} c_i \cdot x^i \in B_\tau$   
**Output:**  $\mathbf{u} = \mathbf{c} \cdot \mathbf{a} = [\mathbf{u}^{(0)}, \dots, \mathbf{u}^{(r-1)}]^T \in R_q^r$ , where  $\mathbf{u}^{(j)} = \mathbf{c} \cdot \mathbf{a}^{(j)} = \sum_{i=0}^{n-1} u_i^{(j)} X^i \in R_q$

```

1: for  $i \in \{0, 1, \dots, n-1\}$  do
2:    $w_i := 0, v_i := 0, v_{i-n} := 0$ 
3:   for  $j \in \{0, 1, \dots, r-1\}$  do
4:      $v_i := v_i \cdot M + (U + a_i^{(j)})$ 
5:      $v_{i-n} := v_{i-n} \cdot M + (U - a_i^{(j)})$ 
6:  $\gamma := 2U \cdot \frac{M^r-1}{M-1}$ 
7: for  $i \in [0, n)$  do
8:   if  $c_i = 1$  then
9:     for  $j \in [0, n)$  do
10:       $w_j := w_j + v_{j-i}$ 
11:   if  $c_i = -1$  then
12:     for  $j \in [0, n)$  do
13:       $w_j := w_j + (\gamma - v_{j-i})$ 
14: for  $i \in \{0, 1, \dots, n-1\}$  do
15:    $t := w_i$ 
16:   for  $j \in \{0, 1, \dots, r-1\}$  do
17:      $u_i^{(r-1-j)} := (t \bmod M) - \tau U \bmod q$ 
18:    $t := \lfloor t/M \rfloor$ 
19: return  $\mathbf{u} = [\mathbf{u}^{(0)}, \dots, \mathbf{u}^{(r-1)}]^T$ 

```

A distinctive feature of the ML-DSA signing procedure is the sparse ternary nature of  $\mathbf{c}$ , and vectors  $\mathbf{s}_1$ ,  $\mathbf{s}_2$ , and  $\mathbf{t}_0$  composed of small-norm polynomials. Specifically, for  $i \in [0, n)$  and  $j \in [0, l)$  for  $\mathbf{s}_1$  or  $[0, k)$  for  $\mathbf{s}_2$ , we have:

- $\mathbf{c}$  is a ternary polynomial where  $c_i$  ranges within  $\{-1, 0, 1\}$ , with only  $\tau$  non-zero coefficients.
- The polynomial coefficients in  $\mathbf{s}_1$  and  $\mathbf{s}_2$  are confined to  $[-\eta, \eta]$ , denoting that  $s_{1,i}^{(j)}, s_{2,i}^{(j)} \in [-\eta, \eta]$ .
- The polynomial coefficients in  $\mathbf{t}_0$  are restricted to  $[-2^{d-1} + 1, 2^{d-1}]$ , a subset of  $[-2^{d-1}, 2^{d-1}]$ .

These properties make conventional NTT approach inefficient for computing  $\mathbf{c} \cdot \mathbf{s}_1$ ,  $\mathbf{c} \cdot \mathbf{s}_2$ , and  $\mathbf{c} \cdot \mathbf{t}_0$ , as it transforms small integers in  $[-\eta, \eta]$  and  $[-2^{d-1}, 2^{d-1}]$  to  $\mathbb{Z}_q$ , where  $\eta$  and  $2^{d-1} \ll q$ , increasing memory usage.

To optimize based on the property, a parallel STPM method has been introduced as an alternative to NTT for Dilithium in [13]. This technique calculates the polynomial multiplications concurrently as detailed in Algorithm 3. The process packs vector  $\mathbf{a}$  into array  $\mathbf{v} := \{v_i\}$ , then stores parallel computation results in array  $\mathbf{w} := \{w_j\}$ , which is derived by summing elements in  $\mathbf{v}$  according to  $c_i$ . Each polynomial multiplication result is extracted by decomposing  $\mathbf{w}$ . Here,  $U$  denotes the upper limit of  $a_i$ ,  $M$  represents multiplicative additions boundary, and  $\gamma$  assists in decomposition. The vector  $\mathbf{a}$  can be substituted by  $\mathbf{s}_1$ ,  $\mathbf{s}_2$ , or  $\mathbf{t}_0$  to determine multiplication outcomes with  $\mathbf{c}$ .

## D. Target Platform

Our focus is high-performance GPU platforms, leveraging their parallel capabilities to enhance signing procedure speed. While CPUs excel at managing the logical flow of general-purpose programs, GPUs are specially designed for tasks requiring intense parallel processing. This design renders GPUs exceptionally effective for computationally demanding tasks, offloading much of the burden traditionally borne by CPUs.

In this architecture, threads execute instructions in streams and can be organized into blocks. Functions that operate on the GPU are termed kernels. A Streaming Multiprocessor (SM) is the primary unit responsible for executing a thread block of a kernel. During execution, blocks are partitioned into warps for single-instruction-multiple-thread execution. Each warp comprises 32 threads with sequential indices.

The GPU memory hierarchy is structured to facilitate rapid data access. Closest to the CUDA cores and also part of each SM are the register file, L1 cache, shared memory, and constant caches, with registers having the fastest access. Beyond these are larger, higher-latency regions shared across all SMs, such as L2 cache, global memory, local memory, texture, and constant memory. Among them, only the register, shared, and global memory support read-write operations, while constant memory is cached in constant caches.

## III. THEORETICAL OPTIMIZATIONS TO ML-DSA SIGNING PROCEDURE

This section details theoretical improvements to the ML-DSA signing procedure. We present our depth-prior optimization, branch elimination strategies, and a refined norm check order, all aimed at enhancing signing efficiency.

### A. Signing Architecture Overview

To provide a clear understanding, we summarize the arithmetic involved. We decompose and reconstruct operations intrinsic to the ML-DSA signing procedure, considering associativity. Fig. 1 presents a detailed graphical representation.

1) CRH: This function refers to a collision resistant hash function that maps to  $\{0, 1\}^{512}$  and is instantiated through SHAKE-256. During signing, it is invoked twice with different inputs, i.e., the concatenated  $tr||M$  and  $K||rnd||\mu$ , to produce the first 64 bytes for  $\mu$  and  $\rho'$ , respectively.

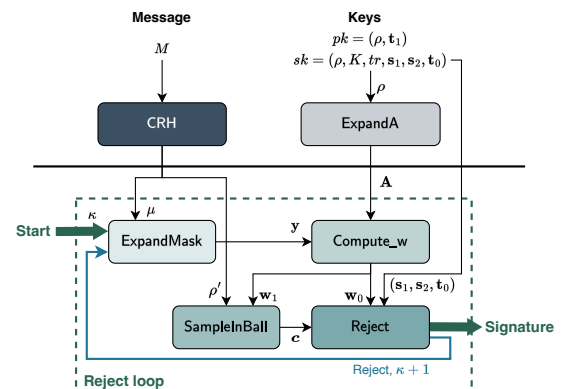


Fig. 1. Structure of the ML-DSA signing procedure.

2) **ExpandA**: This function adopts rejection sampling to sample uniform polynomials and obtain matrix  $\mathbf{A} \in R_q^{k \times \ell}$ . The random streams are generated from  $\rho$  via SHAKE-128. In this process, 3-byte sequences are sequentially extracted and compared against  $q$ , of which that numerically less than  $q$  are retained as coefficients. The derived matrix is interpreted in the NTT domain to enable fast polynomial multiplication.

3) **ExpandMask**: This function employs a principle similar to **ExpandA** but uses SHAKE-256 to generate a random polynomial vector  $\mathbf{y} \in S_{\gamma_1}^\ell$ . As  $\gamma_1$  is a power of 2, rejection does not occur and coefficients are sampled sequentially. The input is the concatenation of  $\rho'$  and  $\kappa$  that introduces randomness to each round. Outputs are generated by taking  $2\gamma_1$  bits as a positive integer and subtracting  $\gamma_1 - 1$  from each result.

4) **Compute\_w**: This process computes the inner-product of matrix  $\mathbf{A}$  and vector  $\mathbf{y}$  to derive  $\mathbf{w} \in R_q^k$ , then decomposes it into high-order and low-order vectors  $\mathbf{w}_1$  and  $\mathbf{w}_0$ . Moreover, a serialization process is invoked on  $\mathbf{w}_1$  in preparation of the subsequent hashing stage.

5) **SampleInBall**: This process uses SHAKE-256 to absorb  $\mu \|\mathbf{w}_1\|$ , yielding  $\tilde{c}$ . The result is then re-input to SHAKE-256 to generate a random stream for  $c$  with  $\tau$  nonzero  $\pm 1$ . The first  $\tau$  bits serve as sign determinants, and  $\tau$  distinct positions in  $[0, n)$  for nonzero values are generate by rejection sampling.

6) **Reject**: This process involves  $sk$ -related computations and checks the resultant value to ensure correctness and avoid secret information disclosure. It computes  $\mathbf{z} := \mathbf{y} + c \cdot \mathbf{s}_1$ ,  $\mathbf{r}_0 := \text{LowBits}_q(\mathbf{w} - c \cdot \mathbf{s}_2)$ , and  $c \cdot \mathbf{t}_0$ . Then it examines if conditions  $\|\mathbf{z}\|_\infty < \gamma_1 - \beta$ ,  $\|\mathbf{r}_0\|_\infty < \gamma_2 - \beta$ , and  $\|c \cdot \mathbf{t}_0\|_\infty < \gamma_2$  are satisfied. Meanwhile, the output  $\mathbf{h}$  of **MakeHint** must meet a hamming weight bound. Any deviation from these conditions results in process abortion and a new iteration begins.

**Potential for Acceleration.** Despite extensive research, further acceleration of the ML-DSA scheme remains possible, particularly in specific scenarios. We discuss potential acceleration strategies below.

1) *Server-oriented design*: In scenarios where a server operates as the subject, two primary strategies emerge to optimize computational efficiency for high-volume signing requests. Firstly, given the server's consistent key, certain key-related operations can be precomputed offline. Secondly, several operations are common across signing tasks and, thus, need not be redundantly executed.

2) *Different multiplication techniques*: During the Reject procedure, one can capitalize on the characteristic that  $c$  is a sparse ternary polynomial. A general NTT approach might overlook this property, leading to inefficiencies. Leveraging specialized multiplication techniques tailored for sparse polynomials can reduce computational complexity and eliminate the need for domain conversions.

3) *Earlier rejection*: In original ML-DSA, a comprehensive polynomial evaluation result must be computed before norm checks begin. By refining the computational pattern, certain coefficients can be determined early, enabling checkpoint inspection and facilitating swifter rejection. Moreover, the conditions to be checked vary in their likelihood of rejection. Prioritizing the assessment of conditions with higher rejection probabilities can further mitigate unnecessary computations.

#### Algorithm 4 Depth-prior sparse ternary polynomial multiplication

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**Input:**  $c = \sum_{i=0}^{n-1} c_i \cdot x^i \in B_\tau$ ,  $a = \sum_{i=0}^{n-1} a_i \cdot x^i \in R_q$   
**Output:**  $u = c \cdot a \in R_q$

```

1: for  $i \in [0, n)$  do
2:    $w_i := 0$ ,  $v_i := a_i$ ,  $v_{i-n} := -a_i$ 
3: for  $j \in [0, n)$  do                                ▷ Traverse polynomial  $a$ 
4:   for  $i \in [0, n)$  do                                ▷ Traverse sparse polynomial  $c$ 
5:     if  $c_i = 1$  then
6:        $w_j := w_j + v_{j-i}$ 
7:     if  $c_i = -1$  then
8:        $w_j := w_j - v_{j-i}$                                 ▷  $w_j$  can be obtained after  $j$ th loop
9: for  $i \in [0, n)$  do
10:   $u_i := w_i \pmod{q}$ 
11: return  $u = \sum_{i=0}^{n-1} u_i \cdot x^i$ 

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In the following, we start from these aspects and propose our optimizations to accelerate the signing of the ML-DSA.

#### B. Depth-Prior Sparse Polynomial Multiplication

The ML-DSA scheme often encounters computational waste when the norms of the resulting values exceed the set bounds. Conventional methods like NTT-based [4], [6] and PSPM-based [13] all face this inefficiency. The applied width-prior approach requires a full polynomial arithmetic operation evaluation before any bounds check can be performed. Motivated by the need to obtain checkable coefficient values more rapidly, we explore a depth-first strategy. This strategy aims to curtail wasteful computations, which is particularly beneficial when the coefficients that exceed the limits have small indices.

Building upon the sparse ternary polynomial multiplication detailed in Algorithm 1, we introduce a depth-prior method depicted in Algorithm 4. The original methodology computes the accumulation on  $w_j$  based on  $c_i$  values, requiring all  $w_j$  values to be determined. In contrast, our approach commences from the  $w_j$  index. For each  $w_j$ , we traverse polynomial  $c$ , accumulating to  $w_j$  according to each  $c_i$  value. This allows some  $w_j$  values to be obtained faster, enabling earlier checks and minimizing potential unnecessary operations. Based on this, we further devise vertical and horizontal parallelism, which improve the entire parallelism of the process to facilitate parallel execution. We give a visualization of our approach and the comparison with NTT-based method in Fig. 2.

**Vertical Parallelism.** Given the bounded coefficient values of the input polynomial  $a$  and a constant  $\tau$ , each  $w_j$  possesses an upper limit linearly related to the coefficient bounds of  $a$ . If the infinity norm is relatively compact, especially compared to machine word size, we can employ packing techniques. This enables bundling multiple polynomials into a single machine word unit, facilitating single-instruction-multiple-data (SIMD) computations. Consequently, this approach allows operations on polynomial vectors to be performed simultaneously, introducing a vertical parallelism approach.

For a given  $\mathbf{a} = [a^{(0)}, \dots, a^{(r-1)}]^T \in R_q^r$ , where  $\|\mathbf{a}^{(j)}\|_\infty = U \ll q$ ,  $j \in [0, r)$ , we utilize a similar construct as in Algorithm 3 to define:

$$v_i^{(j)} = \begin{cases} U + a_i^{(j)}, & i \in [0, n) \\ U - a_{n+i}^{(j)}, & i \in (-n, 0) \end{cases}, j \in [0, r)$$

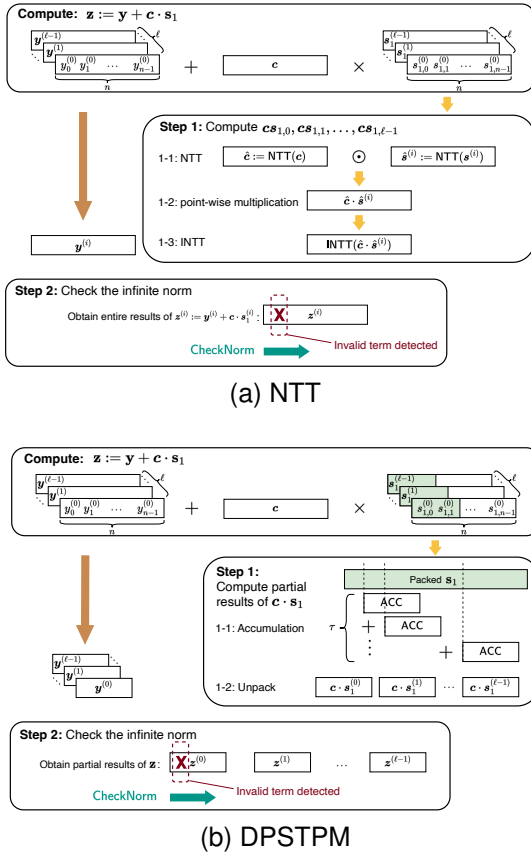


Fig. 2. Comparisons between the (a) NTT and (b) our DPSTPM approach. In (a), the entire result of  $\mathbf{z}$  must be obtained before checking the infinite norm. In (b), the depth-prior approach allows partial results to be checked first, potentially reducing computation when current values are invalid.

Here,  $v_i^{(j)} \in [0, 2U]$ , implying all non-negative values. Consequently, the value of  $w_i^{(j)}$  is constrained to the limit of  $2\tau U$ . Let  $M$  be a power-of-two that satisfies  $M > 2\tau U$ , ensuring that  $2\tau U < M \ll q$ . Given this, we can define:

$$v_i = \begin{cases} (U + a_i^{(r-1)}) \cdot M^{r-1} + \dots + U + a_i^{(0)}, & i \in [0, n) \\ (U - a_{n+i}^{(r-1)}) \cdot M^{r-1} + \dots + U - a_{n+i}^{(0)}, & i \in (-n, 0) \end{cases}$$

Typically, we set  $M = 2^{\lceil \log_2(1+2\tau U) \rceil}$  to simplify implementation through bit-shifting. We discern the upper-bound for  $w_j$  as  $\gamma = 2U \cdot \frac{M^r - 1}{M - 1}$ . Within ML-DSA,  $w_j$  conforms to either 32-bit or 64-bit dimensions, allowing streamlined software representation. After accumulation, we subtract the extraneous  $\tau U$ , with the ultimate result procured via bit-shifting and unpacking. This methodology achieves vertical parallel computation by packing  $r$  polynomial coefficients.

**Horizontal Parallelism.** Since the computation of each  $v_i$  is independent, we introduce horizontal parallelism beyond vertical parallelism, enabling simultaneous computation of multiple  $v_i$  values. This parallelism resembles NTT, where distinct butterfly operations can be executed concurrently. With the computational capabilities of modern systems, such parallelism is readily achievable. For instance, on a GPU, multiple threads can be launched, with each thread handling the computation for a single  $v_i$  or a set thereof.

### Algorithm 5 Depth-prior parallel sparse ternary polynomial multiplication

**Input:**  $(c, \mathbf{a})$ , where  $\mathbf{a} = [a^{(0)}, \dots, a^{(r-1)}]^T \in R_q^r$ , every  $a^{(j)} = \sum_{i=0}^{n-1} a_i^{(j)} \cdot x^i \in R_q$ , and  $c = \sum_{i=0}^{n-1} c_i \cdot x^i \in B_\tau$   
**Output:**  $\mathbf{u} = c \cdot \mathbf{a} = [u^{(0)}, \dots, u^{(r-1)}]^T \in R_q^r$ , where  $u^{(j)} = c \cdot a^{(j)} = \sum_{i=0}^{n-1} u_i^{(j)} \cdot x^i \in R_q$

- 1: **for**  $i \in \{0, 1, \dots, n-1\}$  **do**
- 2:    $w_i := 0, v_i := 0, v_{i-n} := 0$
- 3:   **for**  $j \in \{0, 1, \dots, r-1\}$  **do** ▷ Pack  $r$  coefficients of  $\mathbf{a}$  in  $v$
- 4:      $v_i := v_i \cdot M + (U + a_i^{(j)})$
- 5:      $v_{i-n} := v_{i-n} \cdot M + (U - a_i^{(j)})$
- 6:    $\gamma := 2U \cdot \frac{M^r - 1}{M - 1}$
- 7:   **for**  $j \in \{0, 1, \dots, n-1\}$  **do** ▷ Depth-prior evaluation
- 8:     **for**  $i \in \{0, 1, \dots, n-1\}$  **do**
- 9:       **if**  $c_i = 1$  **then**  $w_j := w_j + v_{j-i}$
- 10:       **if**  $c_i = -1$  **then**  $w_j := w_j + (\gamma - v_{j-i})$
- 11:      $t := w_j$
- 12:     **for**  $i \in (0, 1, \dots, r-1)$  **do** ▷ Unpack to get results
- 13:        $u_{(r-1-i)}^{(j)} := (t \bmod M) - \tau U \bmod q$
- 14:        $t := \lfloor t/M \rfloor$
- 15: **return**  $\mathbf{u} = [u^{(0)}, \dots, u^{(r-1)}]^T$

### Algorithm 6 Unified depth-prior parallel sparse ternary polynomial multiplication

**Input:**  $(c, \mathbf{a})$ , where  $\mathbf{a} = [a^{(0)}, \dots, a^{(r-1)}]^T \in R_q^r$ , every  $a^{(j)} = \sum_{i=0}^{n-1} a_i^{(j)} \cdot x^i \in R_q$ , and  $c = \sum_{i=0}^{n-1} c_i \cdot x^i \in B_\tau$   
**Output:**  $\mathbf{u} = c \cdot \mathbf{a} = [u^{(0)}, \dots, u^{(r-1)}]^T \in R_q^r$ , where  $u^{(j)} = c \cdot a^{(j)} = \sum_{i=0}^{n-1} u_i^{(j)} \cdot x^i \in R_q$

- 1:  $\mathbf{cp} := \{cp_k\}_{k \in [0, \tau)}, j := 0$  ▷ Position array generation phase
- 2: **for**  $i \in [0, n)$  **do**
- 3:   **if**  $c_i = 1$  **then**
- 4:      $cp_j := -i, j = j + 1$
- 5:   **if**  $c_i = -1$  **then**
- 6:      $cp_j := n - i, j = j + 1$
- 7: **for**  $i \in [0, n)$  **do** ▷ Vector packing phase
- 8:    $w_i := 0, v_i := 0, v_{i-n} := 0$
- 9:   **for**  $j \in (0, 1, \dots, r-1)$  **do**
- 10:      $v_i := v_i \cdot M + (U + a_i^{(j)})$
- 11:      $v_{i-n} := v_{i-n} \cdot M + (U - a_i^{(j)})$
- 12:      $v_{i+n} := v_{i+n} \cdot M + (U - a_i^{(j)})$
- 13: **for**  $j \in [0, n)$  **do** ▷ Evaluation phase
- 14:   **for**  $i \in [0, \tau)$  **do**
- 15:      $w_j := w_j + v_{j+cp_i}$
- 16:    $t := w_j$
- 17:   **for**  $i \in [0, r)$  **do** ▷ Results unpacking phase
- 18:      $u_{(r-1-i)}^{(j)} := (t \bmod M) - \tau U \bmod q$
- 19:      $t := \lfloor t/M \rfloor$
- 20: **return**  $\mathbf{u} = [u^{(0)}, \dots, u^{(r-1)}]^T$

### C. Methods for Branch Elimination

In the algorithm described, a remaining concern is the inclusion of branching statements. Notably, while these do not raise side-channel security issues, their presence considerably hinders the potential for code optimization. Branching statements inhibit several compilation-phase optimizations, including loop unrolling and constant folding. Additionally, the unpredictability introduced by these statements disrupts the optimal alignment of pipeline scheduling due to instruction indeterminacy. Further complications arise in multi-threaded parallel systems, where differing execution paths can culminate in challenges like thread divergence. These factors

collectively degrade performance and impede optimal execution, highlighting the need to devise strategies that effectively minimize branching instructions.

To eliminate branching statements within the algorithm, it is pivotal to first elucidate the foundational reasons for their incorporation. The execution logic can be categorized into two predominant pathways, dependent on the values of  $c$ :

- if  $c_i = 1$ ,  $w_j := w_j + v_{j-i}$ ;
- if  $c_i = -1$ ,  $w_j := w_j + (\gamma - v_{j-i})$ .

Here,  $\gamma := 2U \cdot \frac{M^r-1}{M-1}$ . Thus the primary impetus for these branches arises from the heterogeneity in the addends.

To address the complexity introduced by these diverse addends, our preliminary strategy seeks to standardize them. By defining  $\bar{v}_{j-i} = \gamma - v_{j-i}$ ,  $j \in [0, r)$ , we obtain:

$$\bar{v}_i^{(j)} = \begin{cases} (U - a_i^{(r-1)}) \cdot M^{r-1} + \dots + U - a_i^{(0)}, & i \in [0, n) \\ (U + a_{n+i}^{(r-1)}) \cdot M^{r-1} + \dots + U + a_{n+i}^{(0)}, & i \in (-n, 0) \end{cases}$$

By refining the range of  $i$  within this equation, we can incorporate it into the original expression of  $v_i^{(j)}$ . Consequently,

$$v_i^{(j)} = \begin{cases} (U + a_{n+i}^{(r-1)}) \cdot M^{r-1} + \dots + U + a_{n+i}^{(0)}, & i \in [n, 2n) \\ (U - a_i^{(r-1)}) \cdot M^{r-1} + \dots + U - a_i^{(0)}, & i \in [0, n) \\ (U + a_{n+i}^{(r-1)}) \cdot M^{r-1} + \dots + U + a_{n+i}^{(0)}, & i \in (-n, 0) \end{cases}$$

Therefore, the previous branching can be reformulated as:

- if  $c_i = 1$ ,  $w_j := w_j + v_{j-i}$ ;
- if  $c_i = -1$ ,  $w_j := w_j + v_{n+j-i}$ .

One residual challenge lies in the inconsistent index of the addends. To address this, we propose altering the structure of  $c$ . Instead of preserving the complete  $c$  during sampling, we only conserve the respective  $\tau$  positions, thereby mitigating the index variations. Let  $cp$  represent the positions array, thus  $cp_j := -i$  if  $c_i = 1$  and  $cp_j := n - i$  if  $c_i = -1$ . This configuration unifies the accumulation phase expression as  $w_j := w_j + v_{j+cp_i}$ , eliminating the need for branching. A detailed representation of this refined approach is delineated in Algorithm 6.

#### D. Rejection-Prioritized Norm Checking Order

In ML-DSA's signing procedure, four distinct conditions must be met for a valid signature, as shown in Algorithm 2. The initial two conditions stipulate that  $\|\mathbf{z}\|_\infty < \gamma_1 - \beta$  and  $\|\mathbf{r}_0\|_\infty < \gamma_2 - \beta$ . The likelihood of all coefficients meeting these bounds are  $e^{-256 \cdot \beta l / \gamma_1}$  and  $e^{-256 \cdot \beta k / \gamma_2}$ , respectively. The cumulative probability of both conditions being met is  $e^{-256 \cdot \beta (l/\gamma_1 + k/\gamma_2)}$ . Based on the parameter values in Table I, these two conditions primarily dictate rejection process restarts, rather than the conditions encompassing  $\|c \cdot \mathbf{t}_0\|_\infty$  and hints. Furthermore, as  $k/\gamma_2$  typically surpasses  $l/\gamma_1$ ,  $\mathbf{r}_0$  is more susceptible to rejection than  $\mathbf{z}$ . Drawing from this analysis, we advocate for a rejection-prioritized norm checking sequence. In the DPSTPM computation, we commence with  $c \cdot s_2$ , which is attributed with the highest rejection probability, followed sequentially by  $c \cdot s_1$  and  $c \cdot \mathbf{t}_0$ . Implementing this refined norm checking sequence enables early checking of conditions with high rejection probabilities, effectively curtailing redundant execution procedures.

#### E. Discussions of Proposed Methods

Below, we discuss some features of our techniques, including the advantages, novelty, correctness, and security.

**Advantage of Depth-Prior PSTPM.** The principal merit of our method lies in its rapid rejection capability via the depth-prior computational pattern, significantly reducing redundant calculations during the rejection phase. Besides this, our technique offers additional benefits:

- **Multi-dimensional parallelism:** Unlike the singularly horizontal parallelism of NTT, our DPSTPM introduces an additional vertical parallelism dimension. This facilitates simultaneous operations on diverse polynomials even within standard machine word boundaries.
- **Flexibility:** DPSTPM's parallelism boasts inherent adaptability due to its minimal constraints on parallelism degree. Conversely, NTT entails stringent requirements for parameter selection and parallelism degree. Our approach permits an arbitrary number of  $v_i$  computations at once, each functioning independently.
- **Lightweight and constant-time implementation:** Multiplication operations can be burdensome and potentially variable in execution time on lightweight platforms, introducing a risk of side-channel attacks. Our DPSTPM eliminates multiplications, relying solely on lightweight addition and bit-shifting. Additionally, branching only pertains to the public  $c$ , avoiding energy analysis concerns.

**Novelty.** While Dai et al. [23] also applied STPM on GPUs to accelerate NTRU signatures and proposed storing non-zero coefficient positions, our approach has several differences. First, their method uses fixed-size tables due to constant numbers of 1 and -1 coefficients. Second, the different ring setting makes the detail computation different in the accumulation. Additionally, we devise novelty techniques, including the multi-dimensional parallelism and depth-prior computational pattern. Unlike [23], which lacks coefficient packing, our method enables SIMD computation for vertical parallelism. Our ML-DSA-tailored depth-prior computation enhances the rejection process, improving overall performance.

**Effects on Original ML-DSA design.** Our approach only accelerates the detection of invalid signatures without affecting the original design. The checks of  $\|\mathbf{z}\|_\infty < \gamma_1 - \beta$  and  $\|\mathbf{r}_0\|_\infty < \gamma_2 - \beta$  are independent. Valid signatures must satisfy both conditions, while if either is not satisfied, the current value will be rejected and the loop restarted. Therefore, our modification does not affect correctness. Additionally, this modification preserves the nature of the MLWE- and SelfTargetMSIS-based problems. For Unforgeability under Chosen Message Attacks (UF-CMA) security, the adversary must output a valid pair  $(M, (\mathbf{z}, \mathbf{h}, c))$  satisfying  $\|\mathbf{z}\|_\infty < \gamma_1 - \beta$ ,  $\mathcal{H}(\mu \| \text{UseHint}_q(\mathbf{h}, \mathbf{A}\mathbf{z} - c\mathbf{t}_1 \cdot 2^d, 2\gamma_2)) = c$ , and the number of coefficients in  $\mathbf{h}$  equaling 1 being less than  $\omega$ . All these can be satisfied since our method does not change any condition checks. Similarly, the strong UF-CMA can also be proved. For implementation, we apply constant-time techniques to prevent side-channel leakage. Meanwhile, our implementation provides the same test vectors, proving adherence to the original ML-DSA design.



#### IV. SERVER-ORIENTED GPU ACCELERATOR DESIGN

In this section, we introduce cuML-DSA, a tailored GPU accelerator optimized for server-centric environments. We explore the potential benefits under this scenario, and outline a dedicated GPU architecture for the ML-DSA signing and describe several optimization techniques. This encompasses integrating DPSTPM with early evaluation, optimizing memory access, and strategic component caching, collectively culminating in minimized IO latency and heightened performance.

##### A. Design Overview

Our implementation focuses the proposed optimized signing of ML-DSA. Unlike previous works, which used 32 threads [12] or alternated between 32 and 128 threads [11], we allocate a block of 128 threads to each task. This offers significant advantages, including optimal memory access and 100% SM occupancy. In contrast, the 32-thread configuration achieves only 33.3% occupancy. Notably, lower occupancy doesn't always reduce performance. It allows greater use of registers and shared memory, potentially reducing overall IO latency. However, our scenario benefits from the 100% occupancy configuration, which provides sufficient memory resources without sacrificing data access speed. Moreover, [11] shows that several operations are more efficient with 128 threads compared to 32. Based on these, we adhere to the design in Sec III-A and implement corresponding kernels. We also introduce a Pack kernel to preprocess  $sk$  components. Given our server-oriented focus, only  $m$ -related kernels remain online, while ExpandA and Pack kernels are relegated to offline operations.

To efficiently manage multiple signing tasks, we implement batch processing within our kernels for simultaneous task execution. We also adopt the memory pool design from [11] to ensure secure and efficient memory access. Furthermore, we utilize the dynamic scheduling mechanism described in [11] to optimize hardware resource allocation. This approach addresses potential occupancy declines due to varying repetitions across different signing tasks. Consequently, we maintain consistently high occupancy and maximizes hardware utilization.

##### B. Implementation Details

In pursuit of a coherent and streamlined design, we deconstruct the six stages in ML-DSA signing to extract and identify the underlying arithmetic structures. Table II presents a detailed breakdown of each resultant step and its encompassing functions. From this analytical deconstruction, we derive a comprehensive structural design, as illustrated in Fig. 3.

We delineate our GPU implementation of the inline functions below, with pseudocode detailed in Algorithm 7. The inline functions can be stratified into two categories. The first comprises functions that operate singularly on one operand, without requiring data or thread interaction. Every thread processes a single element, invoking the functions to derive the outcomes. The functions within this category include:

1) **ModRed**: We use a variant of Barrett Reduction [6], [24] for modular reduction, replacing division with efficient multiplication and bit-shifting. Unlike the original [24], we compute  $t$  with only addition and bit-shifting, leading to stricter input/output bounds but more effective strategy.

TABLE II  
STRUCTURED DECOMPOSITION OF THE IMPLEMENTED GPU KERNELS AND THE CONSTITUENT INLINE FUNCTIONS.

Kernels	Composing inline functions
CRH	SHAKE
ExpandMask	SHAKE, Serialization
Compute_w	NTT, MontMul, ModRed, Decompose, Serialization
SampleInBall	SHAKE, Sampling
Reject	DPSTPM, CheckNorm, MakeHint, Serialization

##### Algorithm 7 Implementation details of inline functions

```

1: function MontMul( $x \in [-\frac{\nu}{2}, \frac{\nu}{2}], \zeta \in (-q, q)$ )
2:   .reg .s32  $a_h, a_l$   $\triangleright a := a_h \cdot \nu + a_l$ 
3:   mul.hi.s32  $a_h, x, \zeta$ 
4:   mul.lo.s32  $a_l, x, \zeta$   $\triangleright a \leftarrow x \cdot \zeta$ 
5:   mul.lo.s32  $t, a_l, p$   $\triangleright t \leftarrow [a \cdot p]_\nu$ 
6:   mul.hi.s32  $t, t, q$   $\triangleright t \leftarrow t \cdot q/\nu$ 
7:   sub.s32  $t, a_h, t$   $\triangleright a \leftarrow a_h - t$ 
8: function ModRed( $a \leq 2^{31} - 2^{22} - 1$ )
9:    $t := (a + (1 \ll 22)) \gg 23$ 
10:  return  $t := a - t \cdot q$   $\triangleright -6283009 \leq t \leq 6283007$ 
11: function Decompose( $a$ )
12:    $a_1 = (a + 127) \gg 7$ 
13:   # IF  $\gamma_2 == (q - 1)/32$ 
14:    $a_1 = (1025 \cdot a_1 + (1 \ll 21)) \gg 22, a_1 = a_1 \& 15$ 
15:   # ELIF  $\gamma_2 == (q - 1)/88$ 
16:    $a_1 = (11275 \cdot a_1 + (1 \ll 23)) \gg 24$ 
17:    $a_1 = a_1 \wedge (((43 - a_1) \gg 31) \& a_1)$ 
18:    $a_0 = a - 2^{\gamma_2} \cdot a_1$ 
19:    $a_0 = a_0 - (((q - 1)/2 - a_0) \gg 31) \& q$ 
20:  return ( $a_1, a_0$ )
21: function CheckNorm( $a, B$ )
22:    $t := a \gg 31$ 
23:    $t := a - (t \& 2 \cdot a)$ 
24:  return  $1 - ((t - B) \gg 31)$ 
25: function MakeHint( $a_1, a_0$ )
26:  if  $a_0 > \gamma_2 || a_0 < -\gamma_2 || (a_0 = -\gamma_2 \& a_1 \neq 0)$  then
27:    return 1
28:  return 0

```

2) **MontMul**: We leverage Montgomery Reduction [25] to implement modular multiplication. It accepts two integers in the Montgomery domain and yields a result in  $(-q, q)$ . As the product of two 32-bit integers surpasses the register size, we utilize CUDA PTX assembly instructions to optimize register usage and minimize instruction count.

3) **Decompose**: We use macro definitions to encapsulate the two cases of distinct  $\gamma_2$  values in this function. The computation of high- and low- elements adheres to the definitions in [6]. Results are derived using an approximately equal method that ensures constant-time execution and cost-efficiency.

4) **CheckNorm**: This function evaluates  $a$  against the threshold  $B$ . Given the potential negativity, we derive  $|a|$  in constant time using the sign. We obtain the absolute value by masking  $2a$  with the sign and subtracting from  $a$ . The comparison result is discerned from the sign after subtraction.

5) **MakeHint**: This function takes  $(a_1, a_0)$  as input, evaluates three conditions, and subsequently yields the hint bit.

The subsequent category is inherently more intricate, encompassing functions necessitating data interchange, including SHAKE, NTT, and DPSTPM. In implementing SHAKE, we follow the optimized warp-level design as delineated in [11]. The specifics of the remaining functions are elucidated below.

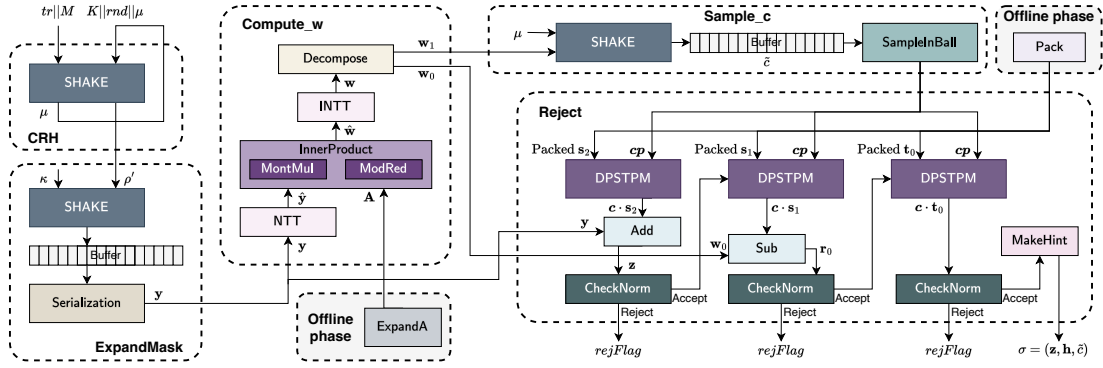


Fig. 3. Architectural design of the ML-DSA signing procedure, segmented by the implemented kernels and comprised of the associated inline functions.

TABLE III  
PARAMETER CONFIGURATION FOR THE DPSTPM IMPLEMENTATION.

Scheme	Operation	$\tau$	$U$	$2\tau U$	$M$	$r$
ML-DSA-44	$c \cdot s_1$	39	2	156	$2^8$	4
	$c \cdot s_2$	39	2	156	$2^8$	4
	$c \cdot t_0$	39	$2^{13}$	638976	$2^{20}$	1
ML-DSA-65	$c \cdot s_1$	49	4	392	$2^9$	5
	$c \cdot s_2$	49	4	392	$2^9$	6
	$c \cdot t_0$	49	$2^{13}$	802816	$2^{20}$	1
ML-DSA-87	$c \cdot s_1$	60	2	240	$2^8$	7
	$c \cdot s_2$	60	2	240	$2^8$	8
	$c \cdot t_0$	60	$2^{13}$	983040	$2^{20}$	1

1) NTT: Unlike [11] that employs both radix-2 and radix-8 approaches, we exclusively employ radix-2 with 128 threads. We store temporary values in shared memory and cache twiddle factors in constant memory. Each thread processes two elements with distance  $2^{8-i}$  at level  $i$ ,  $i \in [1, 8]$ . To prevent performance degradation due to bank conflicts arising from stride memory accesses, we strategically pad bank units, ensuring conflict-free access within identical read/write cycles.

2) DPSTPM: Our implementation focuses on the unified DPSTPM evaluation phase. The function accepts a packed vector  $v$  and position array  $cp$  as inputs and produce evaluation results. We deploy 128 threads and accomplish the evaluation in two rounds. In the  $k$ th round, the  $j$ th thread manages the element  $w_{128k+j}$ , conducting a  $\tau$ -loop that sequentially adds  $v_{128k+j+cp_i}$  to  $w_{128k+j}$ , with  $k \in [0, 2]$ ,  $j \in [0, 128)$ , and  $i \in [0, \tau)$ . Notably, elements accessed by neighboring threads during identical read/write cycles are contiguous, enabling coalesced memory access for maximum speed.

### C. Optimized Reject Kernel

Our implemented kernel for the reject process receives the challenge  $cp$ , the secret key elements, and relevant polynomials as inputs, conducts arithmetic operations over  $R$ , and checks the norms to derive a valid signature. Within this, we incorporate three previously discussed optimizations. First, we employ the DPSTPM algorithm illustrated in Section III-B. Second, we introduce a merging technique that leverages the early evaluation approach. Third, we embrace an order prioritizing  $r_0$  norm-checking for easier rejection. The conventional signing demands numerous NTT and INTT computations.

### Algorithm 8 GPU implementation of DPSTPM with early evaluation for $c \cdot s_2$

**Input:**  $cp, pack_{s_2}$   
**Output:**  $c \cdot s_2$

```

1: shared  $s\_table, s_{s_2}, s_{cp}, s_f$   $\triangleright$  Allocate shared memory
2:  $s_{cp} \leftarrow cp, s_f := 0, reg := 0$ 
3:  $tmp := pack_{s_2}[tid]$ 
4:  $s\_table[tid + N] := tmp$   $\triangleright$  Prepare PSTPM table
5:  $s\_table[tid + N + 128] := tmp$ 
6:  $s\_table[tid], s\_table[tid + 2N] := Mask_{s_2} - tmp$ 
7:  $s\_table[tid + 128], s\_table[tid + 2N + 128] := Mask_{s_2} - tmp$ 
8: for  $j \in [0, \tau)$  do  $\triangleright$  First round DPSTPM evaluation
9:    $idx := tid + s_{cp}[j]$ 
10:   $reg = reg + s\_table[idx]$ 
11: syncthreads()
12: for  $i \in [0, k)$  do
13:   $res := (reg \& Mask_P) - \tau \cdot \eta$ 
14:   $reg := reg \gg Bit_P$ 
15:   $res := w_0[i][tid] - res \bmod q$ 
16:   $rejFlag := \_any\_sync(CheckNorm(\gamma_2 - \beta, res))$ 
17:  if  $lid = 0$  and  $rejFlag = 1$  then
18:     $s_f := 1$ 
19:  syncthreads()
20:  if  $s_f$  then return
21:   $s_{s_2}[i][tid] := res$   $\triangleright$  Write results to shared memory
22: for  $j \in [0, \tau)$  do  $\triangleright$  Second round DPSTPM evaluation
23:   $idx := tid + s_{cp}[j]$ 
24:   $reg = reg + s\_table[idx + 128]$ 
25: syncthreads()
26: for  $i \in [0, k)$  do
27:   $res := (reg \& Mask_P) - \tau \cdot \eta$ 
28:   $reg := reg \gg Bit_P$ 
29:   $res := w_0[i][tid + 128] - res \bmod q$ 
30:   $rejFlag := \_any\_sync(CheckNorm(\gamma_2 - \beta, res))$ 
31:  if  $lid = 0$  and  $rejFlag = 1$  then  $s_f := 1$ 
32:  syncthreads()
33:  if  $s_f$  then return
34:   $s_{s_2}[i][tid + 128] := res$   $\triangleright$  Write results to shared memory
```

Transitioning to the DPSTPM approach reduces multiplications and facilitates the evaluation of multiple polynomials through a singular computation. Combining the depth-first computational mode with this optimized order, we can expedite rejection, thereby curtailing unnecessary computations.

**Merging with Early Evaluation.** We introduce a technique merging DPSTPM with early evaluation to expedite invalid signature rejection, which is compatible with all three evaluation processes. The principle is splitting the evaluation into two rounds. After each round, a sequential unpacking is executed



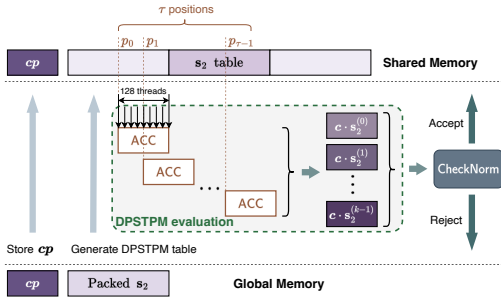


Fig. 4. Optimized memory access pattern for DPSTPM evaluation of  $c \cdot s_2$ .

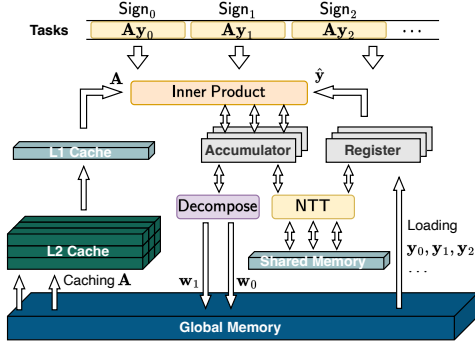


Fig. 5. Layered Caching Strategy for the computation of  $A \cdot y$ .

to derive each half results, followed by arithmetic operations and norm bound assessments. An illustrative implementation of the merged method for computing  $r_0 := w_0 - c \cdot s_2$  and verifying  $\|r_0\|_\infty < \gamma_2 - \beta$  in ML-DSA-44 is detailed in Algorithm 8. Here,  $r = k$ ,  $tid$  represents the thread indices, and  $lid$  signifies the lane indices of threads within a warp, with  $tid \in [0, 128)$  and  $lid \in [0, 32)$ . The procedure commences with generating a table base on  $s_2$  for DPSTPM evaluation. Each thread subsequently undertakes the  $\tau$ -loop for a singular round of evaluation, and then unpacks the  $i$ th polynomial coefficient and subtract it from  $w_0[i][tid]$  to check the norm. Finally, thread states are synchronized to determine if rejection is required, subsequently updating the rejection flag.

**Optimized Memory Access Pattern.** To achieve low latency data access across all evaluations, we allocate  $cp$  and the three DPSTPM tables to shared memory, while frequently accessed accumulators are designated to registers. Unlike other evaluations,  $c \cdot s_2$  needs to be temporarily stored for subsequent computations. Thus, we transfer it from registers to shared memory to maintain balance, as illustrated in Fig. 4. Such an approach presents dual advantages. First, it conserves registers for other computations, reducing the risk of register overuse, which diminish kernel occupancy. Second, it ensures relatively fast access speeds for both writing and retrieving  $c \cdot s_2$ .

#### D. Caching Key Component

In the basic design of the Compute\_w kernel, a 128-thread block is dedicated to manage computations of a signing task. For the inner-product of matrix  $A$  and vector  $y$ , each thread loads two coefficients of both entities from the global memory into the block's specific memory segment. The thread then

performs multiplication and accumulation to complete the computation. Notably, when the server functions as an entity with an invariant key, matrix  $A$  is consistently reloaded across all active blocks. In the architecture of [11], the memory pool segment dedicated to each signing task reserves space for  $A$ , prompting each signing task to load it autonomously. This approach offers no computational advantages during compilation and results in significant memory access overhead.

Leveraging caching for  $A$  presents a potential solution to the issue, but its substantial memory requirements exceed shared memory capacity, especially for larger parameter sets like ML-DSA-65 and ML-DSA-87. To avoid impacting SM occupancy and overall performance, we separate  $A$  from task-specific memory segments and allocate it to a discrete global memory region accessible by all blocks. Under this memory access paradigm, and given the frequent loading patterns, both L2 and L1 caches play pivotal roles in caching the matrix. The comprehensive design is depicted in Fig. 5. In this architecture,  $A$  follows the memory hierarchy, being cached in a stratified manner, transitioning from global memory to L2 and then to L1. Each block loads its associated  $y_i$  to registers to expedite access, given its recurrent use during computations. We allocate  $2k$  registers per thread as accumulators for summative results, with shared memory reserved for NTT and INTT data interchange. Finally, we derive  $w_0$  and  $w_1$  by decomposition, which are then transferred back to global memory.

#### E. Sparse Polynomial Sampler and Adaptations

To cater to both the original sampling method and our DPSTPM strategy, we devise three distinct versions of the sparse polynomial sampler for the sampling of  $c$ .

The first version follows the original procedure, preserving the entire  $c$ . A random stream is generated from  $\tilde{c}$ , with the initial 8 bytes determining signs and the remainder generating positions. However, this approach requires traversing  $c$  to obtain the  $\tau$  positions in DPSTPM. Consequently, our second variant directly archives positions  $cp$  during sampling, omitting the retention of  $c$ . Here, we set  $cp_j := -i$  when  $c_i = 1$  and  $cp_j := n - i$  when  $c_i = -1$ . Nonetheless, both versions are limited in parallel computation potential due to the random nature of the data, which can lead to data conflicts and read/write competition among threads.

Thus, we introduce a third version that allow parallel computations. We construct a Boolean lookup table to track existing positions, thereby ensuring generating  $\tau$  distinct positions. This method eliminates the need for exhaustive comparisons or traversals, which is more efficient and can serve as a complementary solution given it inherently alters test vectors.

### V. PERFORMANCE EVALUATION

#### A. Experimental Setup

The C/C++ source code is compiled utilizing g++ 12.2.0, while the GPU implementation uses CUDA 11.8. All compilations and executions are conducted on an Arch Linux system with kernel 5.15. For CPU benchmarks, we use an Intel(R) XEON W7-2495X CPU with 2.5GHz base frequency. The performance evaluations are performed on a NVIDIA Tesla

TABLE IV

KERNEL PROFILING RESULTS FOR  $(\mathbf{w}_1, \mathbf{w}_0) = \mathbf{A} \cdot \mathbf{y}$  COMPUTATION PRE- AND POST-OPTIMIZATION ACROSS THE THREE ML-DSA PARAMETER SETS. HERE, FMA REPRESENTS THE FUSED MULTIPLY ADD/ACCUMULATE PIPELINE, WHILE ALU DENOTES THE ARITHMETIC LOGIC UNIT.

Parameter Set		ML-DSA-44			ML-DSA-65			ML-DSA-87		
Optimization Method		Before	After	Opt.	Before	After	Opt.	Before	After	Opt.
Execution Time ( $\mu s$ )		69.86	56.64	<b>1.23×</b>	104.64	80.8	<b>1.30×</b>	169.76	119.1	<b>1.43×</b>
Achieved Occupancy (%)		41.59	42.92	<b>+3.19%</b>	38.92	38.99	<b>+0.19%</b>	39.08	39.58	<b>+1.27%</b>
Throughput (%)	Compute	42.39	51.26	<b>+20.91%</b>	38.29	50.18	<b>+31.04%</b>	34.6	48.9	<b>+41.31%</b>
	Memory	47.36	56.89	<b>+20.12%</b>	44.33	55.98	<b>+26.28%</b>	49.08	52.73	<b>+7.44%</b>
Pipeline Utilization (%)	FMA	30.67	38.08	<b>+24.15%</b>	27.98	36.77	<b>+31.43%</b>	22.84	36.08	<b>+57.96%</b>
	ALU	29.16	36.57	<b>+25.39%</b>	26.38	36.63	<b>+38.84%</b>	25.31	36.02	<b>+42.32%</b>
Cache Hit Rate (%)	L1	9.2	57.34	<b>+523.40%</b>	3.21	60.78	<b>+1790.76%</b>	2.14	63.77	<b>+2876.22%</b>
	L2	42.67	72.15	<b>+69.08%</b>	41.7	76.21	<b>+82.76%</b>	38.71	78.31	<b>+102.31%</b>

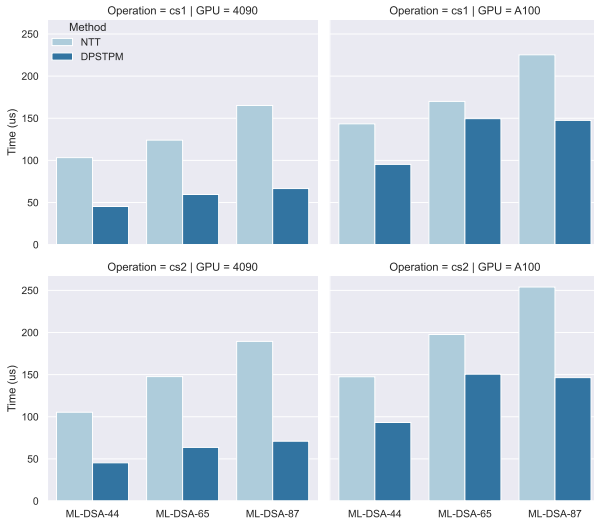


Fig. 6. Performance analysis of batch processing 10,000 executions for  $c \cdot s_1$  and  $c \cdot s_2$ . Vertical parallelism values are  $r = 4, 5, 7$  for  $c \cdot s_1$ , and  $r = 4, 6, 8$  for  $c \cdot s_2$ , across the three respective parameter sets.

TABLE V

EXECUTION TIME OF THREE SPARSE POLYNOMIAL SAMPLERS (MEASURED IN MICROSECONDS ( $\mu s$ )).

Platform	Parameter Set	Sampling Method		
		I	II	III
GeForce RTX 4090	ML-DSA-44	87.52	87.62	71.04
	ML-DSA-65	86.72	87.36	72.54
	ML-DSA-87	101.57	100.32	88.93
Tesla A100	ML-DSA-44	130.85	131.84	115.3
	ML-DSA-65	132.99	133.7	117.63
	ML-DSA-87	159.42	160.19	145.18

A100 80G PCIe and a NVIDIA GeForce RTX 4090. In the experiments, we batch processing 10,000 computational tasks, with execution time recorded in microseconds ( $\mu s$ ). Overall efficiency is represented as throughput in operations per second (OP/s), indicating the number of signatures successfully completed within a second.

### B. Evaluation of Optimization Effectiveness

Below, we undertake a series of experiments to evaluate the efficacy of the proposed methods.

**Comparison of DPSTPM and NTT.** Fig. 6 compares execution times between the NTT approach and our DPSTPM

for  $c \cdot s_1$  and  $c \cdot s_2$  evaluations, which extensively utilize our proposed parallel technique, with vertical parallelism denoted by  $r = k$  or  $l$ , respectively. Performance metrics across both the 4090 and A100 GPUs are presented. For each computation of  $c \cdot s_1$  and  $c \cdot s_2$ , a batch of 10,000 computational tasks is processed. Our DPSTPM consistently surpasses the original NTT method, showcasing execution speed enhancements of 52.0% to 59.7% for  $c \cdot s_1$  and 56.9% to 62.5% for  $c \cdot s_2$ . The A100 GPU shows slightly reduced acceleration effect for ML-DSA-65, primarily attributable to parameter-induced influences on hardware task scheduling. For other parameter sets, the performance enhancement remains between 33.6% and 42.3%. Considering the vertical parallelism, which is  $r = 4, 5, 7$  for  $c \cdot s_1$  and  $r = 4, 6, 8$  for  $c \cdot s_2$  across the three parameter sets, the execution time for  $c \cdot s_2$  is longer than that for  $c \cdot s_1$ , by approximately 4  $\mu s$  on the 4090 GPU. Unlike NTT, the main performance dominant for the DPSTPM is the variable  $\tau$ , which affects both the computational complexity and the entire computation.

**Speedups through Caching.** Table IV presents kernel profiling metrics for the computation  $(\mathbf{w}_1, \mathbf{w}_0) = \mathbf{A} \cdot \mathbf{y}$ , comparing pre- and post-optimization results. The enhancement is primarily due to our refined memory configuration and access strategies. Our approach leverages various classes of on-chip memory based on specific access properties, leading to substantial increases in both L1 and L2 cache hit rates by 2876.22% and 102.31%, respectively. This leads to more efficient memory accesses, reduced execution time, optimized processor resource usage, and improved pipeline scheduling. As our method primarily uses addition and logical operations, there is an increase in the FMA and ALU pipeline utilization. For the ML-DSA-44 parameter set, execution time is reduced from 69.86  $\mu s$  to 56.64  $\mu s$ , yielding a 1.23 $\times$  speedup. Similar enhancements are observed for ML-DSA-65 and ML-DSA-87, with speedups of 1.30 $\times$  and 1.43 $\times$ , respectively.

**Performance of Sampler Variants.** Table V presents execution times for three sparse polynomial samplers, benchmarked on both 4090 and A100 GPU platforms. Specifically, method I is the original method where entire  $c$  is stored, method II represents the variant which stores  $cp$ , whereas method III directly samples positions. The first two methods are incompatible with parallel computing, primarily due to the data conflicts and competition. Comparing across both GPU platforms, method I slightly outperforms II, though III consistently demonstrates superior performance. However,

TABLE VI

THROUGHPUT COMPARISON BETWEEN C, AVX2 IMPLEMENTATIONS, THE GPU APPROACH OF [11], AND OUR IMPLEMENTATION. MEASUREMENTS ARE GIVEN IN OP/S. FOR SPEEDUP METRICS, ONLY THE STREAMING METHOD IS CONSIDERED: THE FIRST LINE INDICATES SPEEDUP RELATIVE TO THE C BASELINE, WHILE THE SECOND DENOTES IMPROVEMENT OVER [11]. THE SAMPLING TECHNIQUE EMPLOYED IS METHOD II.

Parameter Set	CPU		Dilithium [11]		This Work (ML-DSA)						
	Ref	AVX2	A100	4090	CPU <sup>1</sup>	A100			4090		
			Streaming	Streaming		Batching	Streaming	Speedup	Batching	Streaming	Speedup
ML-DSA-44	3,105	14,679	765,855	984,803	3,499 +12.7%	771,943	884,683	284.9× +15.5%	1,049,238	1,080,871	348.1× +9.8%
ML-DSA-65	2,267	9,121	513,468	649,498	2,471 +9.0%	538,742	615,811	271.6× +19.9%	736,109	884,195	390.0× +36.1%
ML-DSA-87	1,618	7,137	396,894	488,006	1832 +13.2%	448,515	540,285	333.9× +36.1%	554,651	785,277	485.3× +60.9%

<sup>1</sup>Performance of the original C implementation integrated with our DPSTPM technique and optimized norm checking order.

TABLE VII

THROUGHPUT COMPARISON OF DILITHIUM IMPLEMENTATIONS ACROSS DIFFERENT PLATFORMS. MEASUREMENTS ARE REPRESENTED IN OP/S. THE THROUGHPUT IS DERIVED FROM THE CYCLE COUNTS, TIMES, AND FREQUENCIES PRESENTED IN THE RESPECTIVE PUBLICATIONS.

Related Work	Dilithium2	Dilithium3	Dilithium5	Platform
[7]	23,256	15,873	10,526	UltraScale+ FPGA
[8]	3,448	2,167	1,977	Artix-7 FPGA
[10]	2,310	1,377	1,044	ARM Cortex-A72
[12]	33,965	14,875	20,396	AGX Xavier GPU

method I necessitates an additional step to generate *cp* in subsequent kernels. This particularity highlights the superior compatibility of method II within our implemented framework.

### C. Overall Performance

Table VI summarizes throughput results of the basic software implementation, GPU implementations from related work of Dilithium [11], and our solutions. We utilize the officially open-source version of ML-DSA<sup>1</sup> to serve as our CPU baseline, containing both a C reference and an AVX2-optimized implementation. The study [11] represents the most recent and highest-performing GPU implementation of Dilithium. For a comprehensive assessment, we executed performance comparison on identical GPU platforms.

We show around 10% speedups on the C implementation with our DPSTPM technique and optimized norm checking order. For GPU performance evaluation, we provide two distinct methodologies include batching and streaming. The batching method processes 10,000 signing tasks in a single batch, while the streaming method initiates 10 CUDA streams, each processing 1,000 signing tasks. The results show a consistent superior performance of the streaming method over batching, primarily due to its ability to hide memory transfer latency. On the 4090 GPU, the streaming approach achieves a 41.6% acceleration relative to batching for the ML-DSA-87. Similarly, on the A100 GPU, it consistently surpasses batching, showing enhancements ranging from 14.3% to 20.5%.

Using the server-grade A100 GPU, our framework exhibits speedups of 284.9×, 271.6×, and 333.9× for the three ML-DSA parameter sets against the C baseline. Similarly, on the consumer-oriented 4090 GPU, our solution achieves accelerations of 348.1×, 390.0×, and 485.3×, respectively. Compared

to the AVX2-optimized method, we achieve speedups ranging from 60.3× to 75.7× on the A100 GPU and 73.6× to 110.0× on the 4090 GPU. While CPU designs can benefit from multi-threaded executions, GPU architectures show superior capability in processing computational tasks concurrently. This capacity enables GPUs to function as efficient co-processors, thereby alleviating the computational burden on CPUs and allowing them to prioritize scheduling tasks.

Furthermore, when benchmarked against the generalized GPU design in [11], our implementation demonstrates improvements of 9.8%, 36.1%, and 60.9% for the three ML-DSA parameter sets on the 4090 GPU. Additionally, we observe enhancements of 15.5%, 19.9%, and 36.1% on the A100 platform. These significant improvements are attributable to our refined signing procedure combined with server-oriented architectural considerations.

Table VII delineates the throughput results derived from several related studies [7], [8], [10], [12] across various computational platforms. The research elucidated in [10] focuses on ARM processors, leveraging the acceleration capabilities of NEON. The work [12] delineates GPU implementations, specifically tailored for the AGX Xavier GPU. Concurrently, the studies [7], [8] concentrate on FPGA-based hardware designs. While there is potential to enhance throughput by allocating more hardware area, GPU implementations often emerge as the preferred choice in server-grade scenarios requiring high-performance and real-time solutions.

## VI. CONCLUSION

In this work, we address a significant gap in GPU-optimized implementations for ML-DSA in server environments. Our tailored, server-centric design, enhanced with novel theoretical optimizations, achieves substantial performance gains. The demonstrated speedups against both CPU benchmarks and existing methods show the effectiveness of our approach. Our work contributes to post-quantum cryptographic deployments and underscores the potential of specialized GPU designs in cryptographic performance. As a future direction, we aim to study the acceleration of other standard post-quantum digital signatures and explore the integration of our design in various protocols to facilitate a seamless post-quantum migration.

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<sup>1</sup><https://github.com/pq-crystals/dilithium/tree/standard>

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