Toward High Performance Matrix Multiplication for Exact Computation

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Motivations

- Matrix multiplication plays a central role in computer algebra.
  algebraic complexity of $O(n^\omega)$ *with* $\omega < 2.3727$ [Williams 2011]

- Modern processors provide many levels of parallelism.
  superscalar, SIMD units, multiple cores

High performance matrix multiplication

✓ numerical computing $=$ classic algorithm $+$ hardware arithmetic

✗ exact computing $\neq$ numerical computing

- algebraic algorithm is not the most efficient ($\neq$ complexity model)
- arithmetic is not directly in the hardware (e.g. $\mathbb{Z}, \mathsf{F}_q, \mathbb{Z}[x], \mathbb{Q}[x, y, z]$).

Outline

1. Matrix multiplication with small integers
2. Matrix multiplication with multi-precision integers
3. Matrix multiplication with polynomials

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Matrix multiplication with small integers

This corresponds to the case where each integer result holds in one processor register :

$$A, B \in \mathbb{Z}^{n\times n} \text{ such that } ||AB||_\infty < 2^s$$

where s is the register size.

Main interests

- ring isomorphism :
  $\rightarrow$ computation over $\mathbb{Z}/p\mathbb{Z}$ is congruent to $\mathbb{Z}/2^s\mathbb{Z}$ when $p(n-1)^2 < 2^s$.
- its a building block for matrix mutiplication with larger integers

Matrix multiplication with small integers

Two possibilities for hardware support :

- use floating point mantissa, i.e. $s = 2^{53}$,
- use native integer, i.e. $s = 2^{64}$.

Using floating point

historically, the first approach in computer algebra [Dumas, Gautier, Pernet 2002]

✓ out of the box performance from optimized BLAS

✗ handle matrix with entries $< 2^{26}$

Using native integers

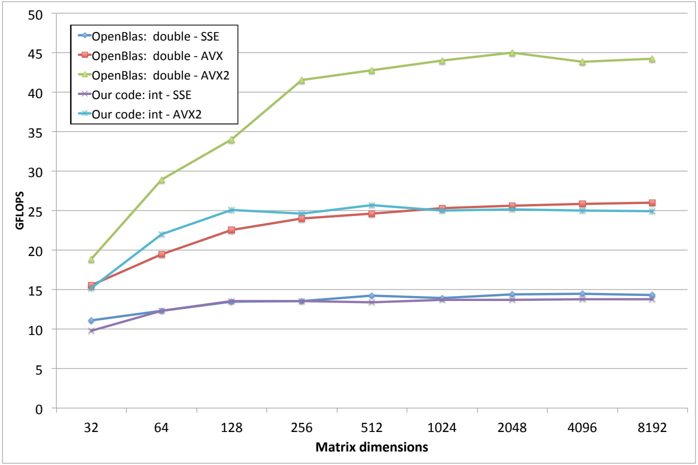
✓ apply same optimizations as BLAS libraries [Goto, Van De Geijn 2008]

✓ handle matrix with entries $< 2^{32}$

Matrix multiplication with small integers

		floating point	integers
Nehalem (2008)	SSE4 128-bits	1 mul+1 add	1 mul+2 add
Sandy Bridge (2011)	AVX 256-bits	1 mul+1 add	
Haswell (2013)	AVX2 256-bits	2 FMA	1 mul+2 add

\# vector operations per cycle (pipelined)



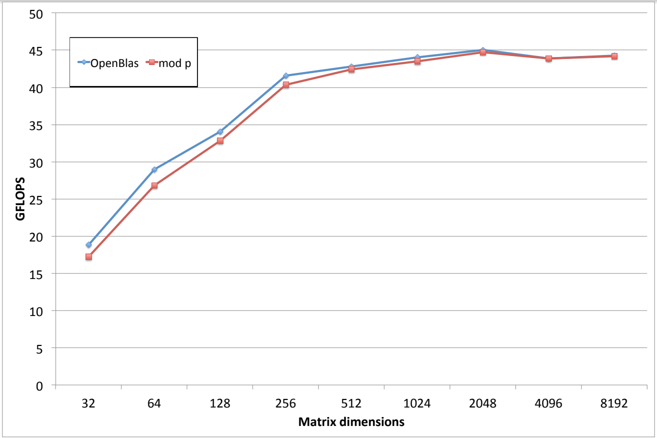
benchmark on Intel i7-4960HQ @ 2.60GHz

Matrix multiplication with small integers

Matrix multiplication modulo a small integer

Let p such that $(p-1)^2 \times n < 2^{53}$

1. perform the multiplication in $\mathbb{Z}$ using BLAS
2. reduce the result modulo p



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Matrix multiplication with multi-precision integers

Direct approach

Let $\mathsf{M}(k)$ be the bit complexity of k-bit integers multiplication and

$$A, B \in \mathbb{Z}^{n\times n} \text{ such that } ||A||_\infty, ||B||_\infty \in \mathsf{O}(2^k).$$

Computing AB using direct algorithm costs $n^\omega \mathsf{M}(k)$ bit operations.

- ✗ not best possible complexity, i.e. $\mathsf{M}(k)$ is super-linear
- ✗ not efficient in practice

<u>Remark</u>:

Use evaluation/interpolation technique for better performances ! ! !

Multi-modular matrix multiplication

Multi-modular approach

$$||AB||_\infty < M = \prod_{i=1}^{k} m_i, \quad \text{with primes } m_i \in O(1)$$

then AB can be reconstructed with the CRT from $(AB) \bmod m_i$.

1. for each m_i compute $A_i = A \bmod m_i$ and $B_i = B \bmod m_i$
2. for each m_i compute $C_i = A_i B_i \bmod m_i$
3. reconstruct $C = AB$ from $(C_1, \ldots, C_k)$

Bit complexity :
$O(n^\omega k + n^2 R(k))$ where $R(k)$ is the cost of reduction/reconstruction

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Bit complexity :
$\mathrm{O}(n^\omega k + n^2 R(k))$ where $R(k)$ is the cost of reduction/reconstruction

- $R(k) = \mathrm{O}(M(k)\log(k))$ using divide and conquer strategy
- $R(k) = \mathrm{O}(k^2)$ using naive approach

Multi-modular matrix multiplication

Improving naive approach with linear algebra

reduction/reconstruction of n^2 data corresponds to matrix multiplication

- ✓ improve the bit complexity from $O(n^2k^2)$ to $O(n^2k^{\omega-1})$
- ✓ benefit from optimized matrix multiplication, i.e. SIMD

Remark :
A similar approach has been used by [Doliskani, Schost 2010] in a non-distributed code.

Multi-modular reductions of an integer matrix

Let us assume $M = \prod_{i=1}^{k} m_i < \beta^k$ with $m_i < \beta$.

Multi-reduction of a single entry

Let $a = a_0 + a_1\beta + \ldots a_{k-1}\beta^{k-1}$ be a value to reduce $\bmod m_i$ then

$$\begin{bmatrix} |a|_{m_1} \\ \vdots \\ |a|_{m_k} \end{bmatrix} = \begin{bmatrix} 1 & |\beta|_{m_1} & \ldots & |\beta^{k-1}|_{m_1} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & |\beta|_{m_k} & \ldots & |\beta^{k-1}|_{m_k} \end{bmatrix} \times \begin{bmatrix} a0 \\ \vdots \\ a_{k-1} \end{bmatrix} - Q \times \begin{bmatrix} m_1 \\ \vdots \\ m_k \end{bmatrix}$$

with $||Q||_\infty < k\beta^2$

Lemma : if $k\beta^2 \in \mathrm{O}(1)$ than the reduction of n^2 integers modulo the m_i's costs $\mathrm{O}(n^2 k^{\omega-1}) + \mathrm{O}(n^2 k)$ bit operations.

Multi-modular reconstruction of an integer matrix

Let us assume $M = \prod_{i=1}^{k} m_i < \beta^k$ with $m_i < \beta$ and $M_i = M/m_i$

$$\text{CRT formulae : } a = \left(\sum_{i=1}^{k} |a|_{m_1} \cdot M_i |M_i^{-1}|_{m_i}\right) \bmod M$$

Reconstruction of a single entry

Let $M_i|M_i^{-1}|_{m_i} = \alpha_0^{(i)} + \alpha_1^{(i)}\beta + \ldots \alpha_{k-1}^{(i)}\beta^{k-1}$ be the CRT constants, then

$$\begin{bmatrix} a_0 \\ \vdots \\ a_{k-1} \end{bmatrix} = \begin{bmatrix} \alpha_0^{(1)} & \ldots & \alpha_{k-1}^{(1)} \\ \vdots & \ddots & \vdots \\ \alpha_0^{(k)} & \ldots & \alpha_{k-1}^{(k)} \end{bmatrix} \times \begin{bmatrix} |a|_{m_1} \\ \vdots \\ |a|_{m_k} \end{bmatrix}$$

with $a_i < k\beta^2$ and $a = a_0 + \ldots + a_{k-1}\beta^{k-1} \bmod M$ the CRT solution.

<u>Lemma</u> : if $k\beta^2 \in O(1)$ than the reconstruction of n^2 integers from their images modulo the m_i's costs $O(n^2 k^{\omega-1}) + \tilde{O}(n^2 k)$ bit operations.

Matrix multiplication with multi-precision integers

Implementation of multi-modular approach

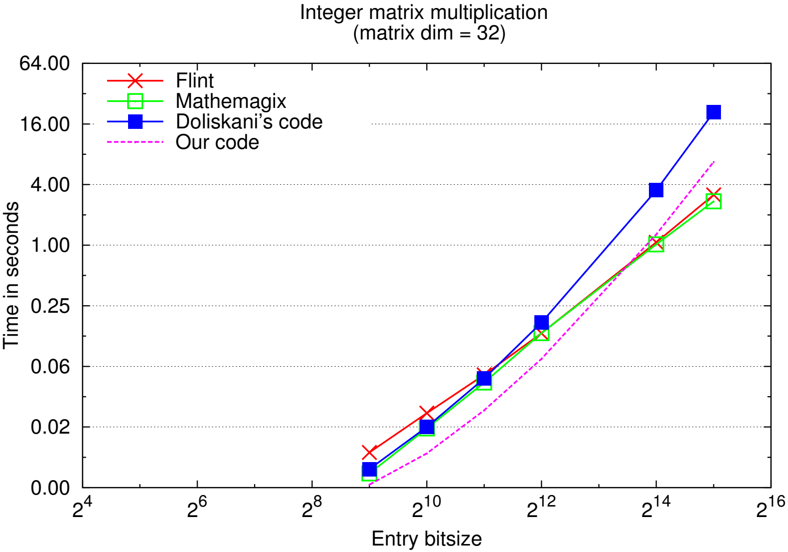
- choose $\beta = 2^{16}$ to optimize β-adic conversions
- choose m_i s.t. $n\beta m_i < 2^{53}$ and use BLAS `dgemm`
- use a linear storage for multi-modular matrices

Compare sequential performances with :

- FLINT library [1] : uses divide and conquer
- Mathemagix library [2] : uses divide and conquer
- Doliskani's code [3] : uses `dgemm` for reductions only

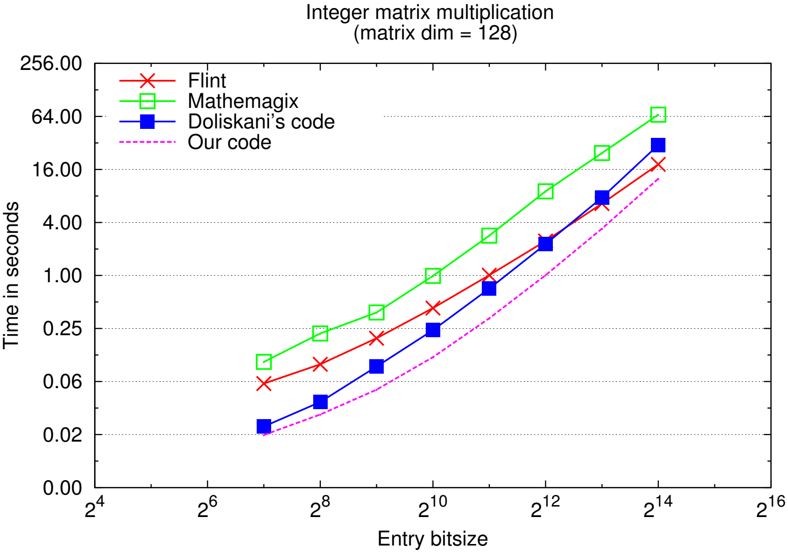
1. www.flintlib.org
2. www.mathemagix.org
3. courtesy of J. Doliskani

Matrix multiplication with multi-precision integers



benchmark on Intel Xeon-2620 @ 2.0GHz

Matrix multiplication with multi-precision integers



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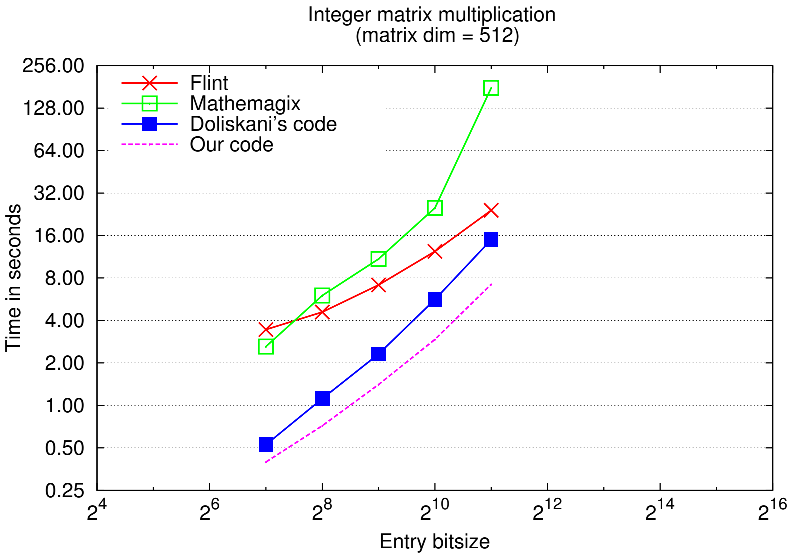

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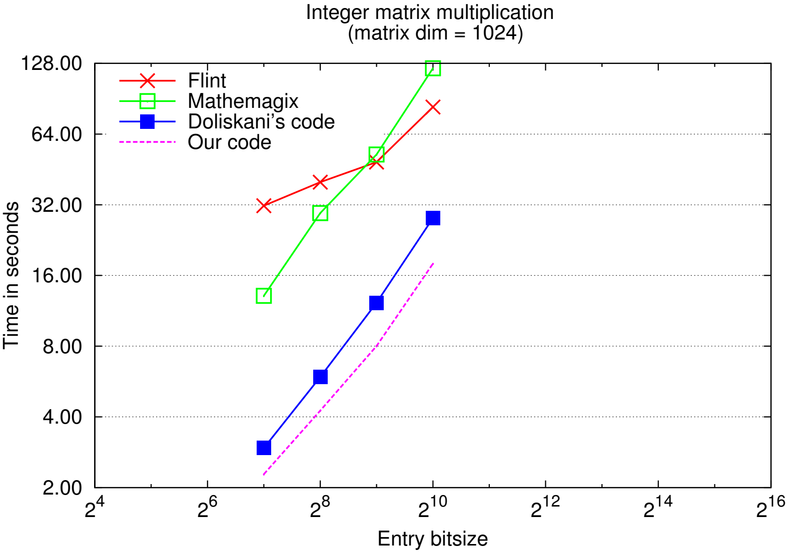

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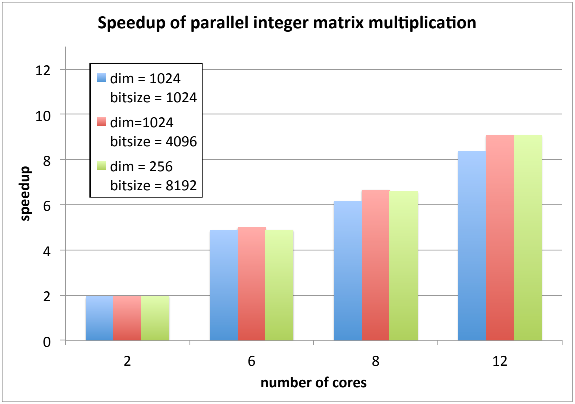
Parallel Matrix multiplication with multi-precision integers

- based on OpenMP task
- CPU affinity (hwloc-bind), allocator (tcmalloc)
- still under progress for better memory strategy ! ! !



benchmark on Intel Xeon-2620 @ 2.0GHz (2 NUMA with 6 cores)

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Matrix multiplication over $\mathrm{F_p[x]}$

We consider the "easiest" case :

$$A, B \in \mathrm{F_p[x]^{n\times n}} \text{ such that } \mathrm{deg(AB) < k = 2^t}$$

- p is a Fourier prime, i.e. $p = 2^t q + 1$
- p is such that $n(p-1)^2 < 2^{53}$

Complexity

$O(n^\omega k + n^2 k \log(k))$ op. in $\mathrm{F_p}$ using evaluation/interpolation with FFT

Matrix multiplication over $\mathsf{F_p[x]}$

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Remark:

using Vandermonde matrix on can get a similar approach as for integers, i.e. $\mathsf{O}(n^\omega k + n^2 k^{\omega-1})$

Matrix multiplication over $\mathsf{F_p}[x]$

Evaluation/Interpolation scheme

Let θ a primitive kth root of unity in $\mathsf{F_p}$.

1. for $i = 1 \ldots k$ compute $A_i = A(\theta^{i-1})$ and $B_i = B(\theta^{i-1})$
2. for $i = 1 \ldots k$ compute $C_i = A_i B_i \in \mathsf{F_p}$
3. interpolate $C = AB$ from $(C_1, \ldots, C_k)$

- steps 1 and 3 : $\mathrm{O}(n^2)$ call to $\mathtt{FFT}_k$ over $\mathsf{F_p}[x]$
- step 2 : k matrix multiplications modulo a small prime p

FFT with SIMD over F_p

Butterly operation modulo p

compute $X + Y \bmod p$ and $(X - Y)\theta^{2^i} \bmod p$.

- Barret's modular multiplication with a constant (NTL)
- calculate into $[0, 2p)$ to remove two conditionals [Harvey 2014]

Let $X, Y \in [0, 2p), W \in [0, p), p < \beta/4$ and $W' = \lceil W\beta/p \rceil$.

Algorithm: Butterfly(X,Y,W,W',p)

1: $X' := X + Y \bmod 2p$
2: $T := X - Y + 2p$
3: $Q := \lceil W'T/\beta \rceil$ — 1 high short product
4: $Y' := (WT - Qp) \bmod \beta$ — 2 low short products
5: return (X', Y')

FFT with SIMD over F_p

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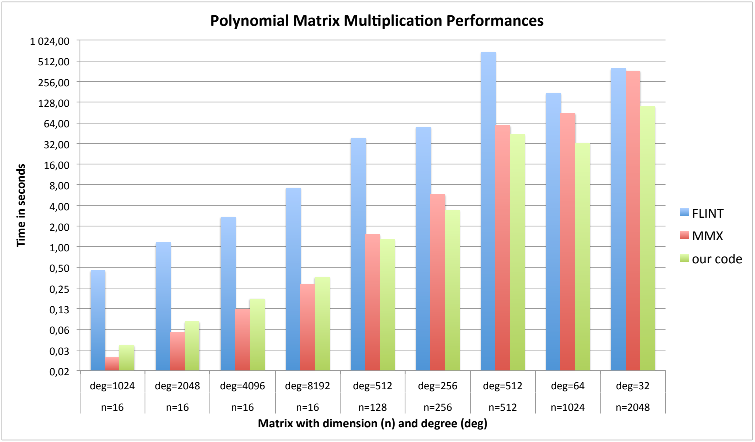
✓ SSE/AVX provide 16 or 32-bits low short product

✗ no high short product available (use full product)

Matrix multiplication over $F_p[x]$

Implementation

- radix-4 FFT with 128-bits SSE (29 bits primes)
- BLAS-based matrix multiplication over F_p [FFLAS-FFPACK library]



benchmark on Intel Xeon-2620 @ 2.0GHz

Matrix multiplication over $\mathbb{Z}[x]$

$A, B \in \mathbb{Z}[x]^{n\times n}$ such that $\deg(AB) < d$ and $||(AB)_i||_\infty < k$

Complexity

- $\tilde{O}(n^\omega d \log(d) \log(k))$ bit op. using Kronecker substitution
- $\mathrm{O}(n^\omega d \log(k) + n^2 d \log(d) \log(k))$ bit op. using CRT+FFT

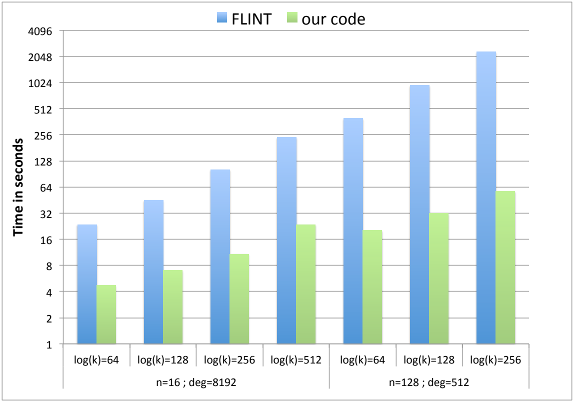
Remark:

if the result's degree and bitsize are not too large, CRT with Fourier primes might suffice.

Matrix multiplication over $\mathbb{Z}[x]$

Implementation

- use CRT with Fourier primes
- re-use multi-modular reduction/reconstruction with linear algebra
- re-use multiplication in $F_p[x]$



benchmark on Intel Xeon-2620 @ 2.0GHz

Parallel Matrix multiplication over $\mathbb{Z}[x]$

Very first attempt (work still in progress)

- parallel CRT with linear algebra (same code as in $\mathbb{Z}$ case)
- perform each multiplication over $F_p[x]$ in parallel
- some part of the code still sequential

n	d	$\log(k)$	6 cores	12 cores	time seq
64	1024	600	$\times 3.52$	$\times 4.88$	61.1s
32	4096	600	$\times 3.68$	$\times 5.02$	64.4s
32	2048	1024	$\times 3.95$	$\times 5.73$	54.5s
128	128	1024	$\times 3.76$	$\times 5.55$	53.9s

Conclusion

High performance tools for exact linear algebra :

- matrix multiplication through floating points
- multi-dimensional CRT
- FFT for polynomial over wordsize prime fields

We provide in the LinBox library (`www.linalg.org`)

- efficient sequential/parallel matrix multiplication over $\mathbb{Z}$
- efficient sequential matrix multiplication over $\mathrm{F_p}[x]$ and $\mathbb{Z}[x]$

Parallel multi-modular matrix multiplication

1. for $i = 1 \ldots k$ compute $A_i = A \bmod m_i$ and $B_i = B \bmod m_i$
2. for $i = 1 \ldots k$ compute $C_i = A_i B_i \bmod m_i$
3. reconstruct $C = AB$ from $(C_1, \ldots, C_k)$

Parallelization of multi-modular reduction/reconstruction

each thread reduces (resp. reconstructs) a chunk of the given matrix

thread 0 | thread 1 | thread 2 | thread 3

$A_0 = A \bmod m_0$

$A_1 = A \bmod m_1$

$A_2 = A \bmod m_2$

$A_3 = A \bmod m_3$

$A_4 = A \bmod m_4$

$A_5 = A \bmod m_5$

$A_6 = A \bmod m_6$

Parallel multi-modular matrix multiplication

1. for $i = 1 \dots k$ compute $A_i = A \bmod m_i$ and $B_i = B \bmod m_i$
2. for $i = 1 \dots k$ compute $C_i = A_i B_i \bmod m_i$
3. reconstruct $C = AB$ from $(C_1, \dots, C_k)$

Parallelization of modular multiplication

each thread computes a bunch of matrix multiplications $\bmod m_i$

thread 0	$C_0 = A_0 B_0 \bmod m_0$
	$C_1 = A_1 B_1 \bmod m_1$
thread 1	$C_2 = A_2 B_2 \bmod m_2$
	$C_3 = A_3 B_3 \bmod m_3$
thread 2	$C_4 = A_4 B_4 \bmod m_4$
	$C_5 = A_5 B_5 \bmod m_5$
thread 3	$C_6 = A_6 B_6 \bmod m_6$