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ISSAC 2014 Software demo

Plan



- 2 Fast Fourier Transform
- 3 ModularPolynomial
- 4 IntegerPolynomial
- 5 RationalNumberPolynomial



Background

Reducing everything to multiplication

- Polynomial multiplication and matrix multiplication are at the core of many algorithms in symbolic computation.
- Algebraic complexity is often estimated in terms of multiplication time
- At the software level, this reduction is also common (Magma, NTL)
- Can we do the same for fork-join-multithreaded algorithms?

Building blocks in scientific software

- The *Basic Linear Algebra Subprograms* (BLAS) is an inspiring and successful project providing low-level kernels in linear algebra, used by LINPACK, LAPACK, MATLAB, Mathematica, Julia (among others).
- Other BB's successful projects: FFTW, SPIRAL (among others).
- The GNU Multiple Precision Arithmetic Library project plays a similar role for rational numbers and floating-point numbers.
- No symbolic computation software dedicated to *sequential* polynomial arithmetic managed to play the unification role of the BLAS.
- Could this work in the case of hardware accelerators?

Functionalities

- Level 1: basic arithmetic operations that are specific to a polynomial representation or a coefficient ring: multi-dimensional FFTs/TFTs, univariate real root isolation
- Level 2: basic arithmetic operations for dense or sparse polynomials with coefficients in Z, Q or Z/pZ.
- Level 3: advanced arithmetic operations taking as input a zero-dimensional regular chains: normal form of a polynomial, multivariate real root isolation.

BPAS Mandate (2/2)

Targeted architectures

- Multi-core processors with code written in CilkPlus or OpenMP. Our Meta_Fork framework performs automatic translation between the two as well as conversions to C/C++.
- Graphics Processing Units (GPUs) with code written in CUDA, provided by CUMODP.
- Unifying code for both multi-core processors and GPUs is conceivable (see the SPIRAL project) but highly complex (multi-core processors enforce memory consistency while GPUs do not, etc.)



Design

Algorithm choice

- Level 1 functions (n-D FFTs/TFTs) are highly optimized in terms of locality and parallelism.
- Level 2 functions provide a variety of algorithmic solutions for a given operation (polynomial multiplication, Taylor shift, etc.)
- Level 3 functions combine several Level 2 algorithms for achieving a given task.

Implementation techniques

- At Level 1, code generation at installation time (auto-tuning) is used.
- At Level 2, the user can choose between algorithms minimizing work and algorithms maximizing parallelism.
- At Level 3, this leads to adaptive algorithms that select appropriate Level 2 functions depending on available resources (number of cores, input data size).

Organization

Developer view point

- Source tree has two branches: 32bit and 64bit arithmetic with large bodies of common code
- Four sub-projects: ModularPolynomial, IntegerPolynomial, RationalNumberPolynomial and Polynomial.
- For the former three, the base ring is known at compile time while the latter provides polynomial arithmetic over an arbitrary BPAS ring.
- Python scripts generate 1-D FFT code at installation time.
- Dense representations, SLPs and sparse representations are available.

User view point today

- Only the 64bit arithmetic branch, but full access to each sub-project.
- Regression tests and benchmark scripts are also distributed.
- Documentation is generated by doxygen.
- A manually written documentation is work in progress.

User interface (1/2)



Figure: A snapshot of BPAS algebraic data structures.

User interface (2/2)

```
#include <bpas.h>
int main(int argc, char *argv[]) {
        /* Univariate Integer Polynomial Multiplication */
        DUZP a(128), b(128);
        a.read("a input.dat"); b.read("b input.dat");
        DUZP c = a * b;
        /* Real Root Isolation */
        mpg class width(1, 20);
        RegularChains rcs;
        rcs.read("rcs input.dat");
        Intervals boxes = realRootIsolation(rcs, width);
        return 0;
}
```

Figure: A snapshot of BPAS code.

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BPAS 1-D FFT

- BPAS 1-D FFTs code is optimized in terms of cache complexity and register usage, following principles introduced by FFTW and SPIRAL.
- The FFT of a vector of size *n* is computed in a divide-and-conquer manner until the vector size is smaller than a threshold, at which point FFTs are computed using a tiling strategy.
- At compile time, this threshold is used to generate and optimize the code. For instance, the code of all FFTs of size less or equal to HTHRESHOLD are decomposed into blocks (typically performing FFTs on 8 or 16 points) for which straight-line program (SLP) machine code is generated by python scripts.
- Instruction level parallelism (ILP) is carefully considered: vectorized instructions are explicitly used (SSE2, SSE4) and instruction pipeline usage is highly optimized.
- Other environment variables are available for the user to control different parameters in the code generation.

1-D FFT Benchmarks



Figure: One-dimensional modular FFTs: Modpn vs BPAS.

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2-D TFT versus 2-D FFT



Figure: Timing of bivariate multiplication for input degree range of [1024, 2048) on 8 cores.

Balanced Dense Multiplication over $\mathbb{Z}/p\mathbb{Z}$



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Integer polynomial multiplication

• Five different integer polynomial multiplication algorithms are available:

Schönhage-Strassen, 8-way Toom-Cook, 4-way Toom-Cook, divide-and-conquer plain multiplication and the two-convolution method.

- The first one has optimal work (among the five) but is purely serial due to the difficulties of parallelizing 1D FFTs on multicore processors.
- The next three algorithms are parallelized but their parallelism is static, that is, independent of the input data size; these algorithms are practically efficient when both the input data size and the number of available cores are small, for details.
- The fifth algorithm relies on modular 2D FFTs which are computed by means of the row-column scheme; this algorithm delivers a high scalability and can fully utilize fat computer nodes.

KS+GMP: Reduction to GMP via Kronecker substitution

•
$$f(x) := \sum_{i=0}^{n} f_i x^i$$
, $g(x) := \sum_{i=0}^{m} g_i x^i$, $h(x) = f(x) \times g(x) = \sum_{i=0}^{n+m-1} h_i x$

• Assume $0 \le f_i < H_f$ and $0 \le j < m$ for all f_i 's and g_j 's.

- Then we have: $0 \le h_k < \min(n, m)H_fH_g + 1$, for $0 \le k < n + m 1$. Thus $B := \lceil \log_2 \min(n, m)H_fH_g + 1 \rceil$ is the maximum number of bits required for representing a coefficient of the result.
- If f or g has a negative coefficient we use a "two-complement"-trick.

Steps

9 Evaluation:
$$Z_f = \sum_{i=0}^n f_i 2^{iB}, \ Z_g = \sum_{i=0}^m f_i 2^{iB}$$

3 Multiplying:
$$Z_h = Z_f \times Z_g$$
 using GMP library.

3 Unpacking:
$$h_i$$
s from $Z_h = \sum_{i=1}^{n+m-1} h_i 2^{iB}$

Analysis

Work is in O(slog(s)log(log(s))). *s* is the maximum bit size of *f* or *g* (Schönhage & Strassen). But no parallelism and modest data locality.

DnC+KS+GMP: GMP Reduction via KS and distributivity

Steps

- O Divide: $f(x) = f_0(x) + x^{n/2}f_1(x)$, $g(x) = g_0(x) + x^{n/2}g_1(x)$ Execute 4 sub-problems recursively.
 - Store $f_0 \times g_0$ and $f_1 \times g_1$ in the result array.
 - Store $f_0 \times g_1$ and $f_1 \times g_0$ in auxiliary arrays.
- O Add the auxiliary arrays to the result.
- Use (one or) two DnC levels, then use the KS+GMP algorithm.

Analysis

Work is in $O(s\log(s)\log(\log(s)))$. But, w.r.t. pure KS+GMP, the constant has increased by approximately by 4. However, parallelism is close to 16.

k-way Toom-Cook and reduction to GMP (1/4)

- **Division**: Write $f(x) = f_0(x) + x^{n/k} f_1(x) + \ldots + x^{(k-1)n/k} f_{k-1}(x)$ and $g(x) = g_0(x) + x^{n/k} g_1(x) + \ldots + x^{(k-1)n/k} g_{k-1}(x)$
- **2** Conversion: Set $X = x^{n/k}$ and apply KS to the f_i 's and g_j 's. Obtaining $F(X) = Z_{f_0} + Z_{f_1}X + \ldots + Z_{f_{k-1}}X^{k-1}$ and $G(X) = Z_{g_0} + Z_{g_1}X + \ldots + Z_{g_{k-1}}X^{k-1}$.
- **Solution**: Evaluate f, g at 2k 1 points: $(0, X_1, \ldots, X_{2k-3}, \infty)$
- **3** Multiplying: $(w_0, ..., w_{2k-2}) = (F(0) \cdot G(0), ..., F(\infty) \cdot G(\infty))$
- Interpolation: recover $(Z_{h_0}, Z_{h_1}, \dots, Z_{h_{2k-2}})$ where: $H(X) = f(X)g(X) = Z_{h_0} + Z_{h_1}X + \dots + Z_{h_{2k-2}}X^{2k-2}.$
- Conversion: recover polynomial coefficients from Z_{h0},..., Z_{h2k-2}.
 Obtaining h(x) = h₀(x) + x^{n/k}h₁(x) + ... + x^{(2k-2)n/k}h_{2k-2}(x).
- Ø Merge: Add intermediate results to the final result.

k-way Toom-Cook and reduction to GMP (2/4)

Parallelization

All steps must be parallelized. For the evaluation and interpolation, we use the fact that these steps can be done via linear algebra.



Calculations are distributed among workers.

k-way Toom-Cook and reduction to GMP (3/4)

Analysis

- Work in O(slog(s)log(log(s))). W.r.t. pure KS+GMP, for k = 8, the constant has increased approximately by 2 for s = 2²⁴.
- However, parallelism is about 7 and 13 when k = 4 and k = 8, resp.
- In the 3 tables below, a 12-core (Intel Xeon) is used.
- In the last one, we have $\sqrt{s} = 8192$.

Toom-o Promea results						
Div. & Conv.	Eval.	Mul.	Inter.	Con. & Merge		
10%	8%	44%	25%	9%		
9%	9%	43%	27%	10%		
8%	8%	45%	28%	9%		
	Div. & Conv. 10% 9% 8%	Div. & Conv. Eval. 10% 8% 9% 9% 8% 8%	Div. & Conv. Eval. Mul. 10% 8% 44% 9% 9% 43% 8% 8% 45%	Div. & Conv. Eval. Mul. Inter. 10% 8% 44% 25% 9% 9% 43% 27% 8% 8% 45% 28%		

Toom-8 Profiled results

	Toom-4 Profiled results						
	\sqrt{s}	Div. & Conv.	Eval.	Mul.	Inter.	Con. & Merge	
1	.6384	13%	3%	57%	11%	13%	
3	82768	12%	3%	61%	11%	12%	
6	5536	8%	2%	66%	10%	11%	

Algorithm	Timing	Work	Span	Work/serial	Span/serial
KS (Ser.)	1	16781990263	16781990263	1	1
DnC	15.86	67222430575	4237755216	4	0.25
Toom-4	6.42	28289430113	4382572841	1.68	0.26
Toom-8	11.26	24449014227	2023790230	1.45	0.12

Notes

• Span of Toom-8 is the best, 12 % of the KS

 \rightarrow It should be much better on better machines.

- Work of the Toom-8 & Toom-4 are more than KS, but much better than DnC.
- But for Toom-8 and Toom-4, GMP-multiplication is not the dominant part.
- Hence, we need an algorithm which can scale on fatter nodes.

Two-convolution method (1/7)

Specifications

- Input: a(y), b(y) ∈ Z[y] with max(deg(a), deg(b) < d and N₀ the maximum bit size of a coefficient among a(y) and b(y).
- Intention: a(y), b(y) are dense in the sense that most coefficients have a size in the order of N_0 .
- **Output**: c(y) = a(y)b(y).

Theorem

Let *w* be the number of bits of a machine word. There exist positive integers N, K, M, with N = K M and $M \le w$, such that the integer N is *w*-smooth (and so is *K*), we have $N_0 < N \le N_0 + \sqrt{N_0}$ and the following algorithm for multiplying a(y), b(y) has

- a work of $O(d K \log_2(d K) (\log_2(d K) + 2M))$ word operations,
- a span of $O(K \log_2(d) \log_2(d K))$ word operations and,
- incurs $O(\lceil dN/wL \rceil + \lceil (\log_2(dK) + 2M) \rceil dK/L)$ cache misses,

Two-convolution method (2/7)

Principle

- **Convert-in**: convert the integer coefficients of a(y), b(y) to $\mathbb{Z}[x]$, thus converting a(y), b(y) to A(x, y), B(x, y) s.t. for some $\beta \in \mathbb{Z}$:
 - $a(y) = A(\beta, y)$ and $b(y) = B(\beta, y)$,
 - **2** $\deg(A, y) = \deg(a)$ and $\deg(B, y) = \deg(b)$,
 - **3** $\max(\text{bitsize}(a), \text{bitsize}(b)) \in \Theta(\max(\text{bitsize}(a), \text{bitsize}(b)))$

Let m > 4H be an integer, where H is the maximum absolute value of a coefficient of the integer polynomial C(x, y) := A(x, y)B(x, y).

- **Compute**: *m* and A(x, y), B(x, y) are constructed such that
 - the polynomials $C^+(x, y) := A(x, y)B(x, y) \mod \langle x^K + 1 \rangle$ and $C^-(x, y) := A(x, y)B(x, y) \mod \langle x^K - 1 \rangle$ are computed over $\mathbb{Z}/m\mathbb{Z}$ via FFT techniques
 - 2 meanwhile the following equation holds over \mathbb{Z} :

$$C(x,y) = \frac{C^+(x,y)}{2}(x^K-1) + \frac{C^-(x,y)}{2}(x^K+1).$$

• Convert-out: Compute $u(y) := C^+(\beta, y)$ and $v(y) := C^-(\beta, y)$ over \mathbb{Z} . Then, deduce $c(y) := \frac{u(y)+v(y)}{2} + \frac{-u(y)+v(y)}{2} 2^N$ over \mathbb{Z} .

Two-convolution method (3/7)



Figure: Multiplication scheme for dense univariate integer polynomials.

Two-convolution method (4/7)

Principle (recall)

- Convert-in: convert a(y), b(y) to A(x, y), B(x, y) s.t. for some $\beta \in \mathbb{Z}$ we have $a(y) = A(\beta, y)$ and $b(y) = B(\beta, y)$.
- 2 Let m > 4H where $H := || C(x, y) ||_{\infty}$ with C(x, y) := A(x, y)B(x, y).
- Compute: $C^+(x, y) := A(x, y)B(x, y) \mod \langle x^K + 1 \rangle$ and $C^-(x, y) := A(x, y)B(x, y) \mod \langle x^K 1 \rangle$ over $\mathbb{Z}/m\mathbb{Z}$.
- Convert-out: Compute $u(y) := C^+(\beta, y)$ and $v(y) := C^-(\beta, y)$ over \mathbb{Z} . Then, deduce $c(y) := \frac{u(y)+v(y)}{2} + \frac{-u(y)+v(y)}{2} 2^N$ over \mathbb{Z} .

Remarks

- For polynomials with size in the Giga-bytes, we can choose m < 2w. Thus each of C⁺(x, y) and C⁻(x, y) requires at most two 2-D FFT/TFT over a prime field with characteristic of machine word size.
- **Convert-in** and **Convert-out** are done only with addition and shift operations on byte vectors: GMP is not used.
- The cache complexity of this process is proved to be optimal.

Two-convolution method (5/7)

\sqrt{s}	ConvertIn	TwoConvolution	ConvertOut	Total
2048	0.038	0.106	0.042	0.195
4096	0.039	0.23	0.107	0.39
8192	0.119	0.895	0.267	1.298
16384	0.248	3.705	0.665	4.643
32768	0.943	16.272	4.217	21.496

Table: Using 2 primes on a 48-core AMD Opteron node.

\sqrt{s}	ConvertIn	TwoConvolution	ConvertOut	Total
2048	0.037	0.113	0.052	0.227
4096	0.028	0.206	0.103	0.364
8192	0.07	0.652	0.307	1.059
16384	0.224	2.71	0.73	3.698
32768	0.943	11.796	4.174	16.978

Table: Using 3 primes on a 48-core AMD Opteron node.

This about four faster than Toom-8 at $\sqrt{s} = 8192$.

Two-convolution method (6/7)



Degree = Maximum bit size of a coefficient

Figure: Dense integer polynomial multiplication: BPAS vs FLINT vs Maple 18.

Two-convolution method (7/7)



Degree << Maximum bit size of a coefficient

Figure: Dense integer polynomial multiplication: BPAS vs FLINT vs Maple 18.

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Univariate Real Root Isolation Algorithm: Find Roots

Input: A univariate squarefree polynomial $f(x) = c_d x^d + \cdots + c_1 x + c_0$ with rational number coefficients

Output: A list of pairwise disjoint intervals $[a_1, b_1], \ldots, [a_e, b_e]$ with rational endpoints such that

- each $[a_i, b_i]$ contains one and only one real root of f(x);
- if $a_i = b_i$, the real root $x_i = a_i (b_i)$; otherwise, the real root $a_i < x_i < b_i (f(x) \text{ doesn't vanish at either endpoint})$.



Figure: An example of input / output

Real Root Isolation (Collins-Vincent-Akritas Algorithm)

Algorithm 1: NumberInZeroOne(p)

Input: a squarefree univariate polynomial p**Output**: number of real roots of p in (0, 1)**begin**

$$\begin{array}{l} p_1 := x^n p(1/x); \ p_2 := p_1(x+1) \\ \text{let } d \text{ be the number of sign variations of the coefficients of } p_2 \\ \textbf{if } d \leq 1 \textbf{ then return } d \\ p_1 := 2^n p(x/2); \ p_2 := p_1(x+1) \\ \textbf{if } x \mid p_2 \textbf{ then } m := 1 \textbf{ else } m := 0 \\ m' := \text{NumberInZeroOne}(p_1) \\ m := m + \text{NumberInZeroOne}(p_2) \\ \text{return } m + m' \\ \textbf{end} \end{array}$$

The Taylor shift $f(x) \mapsto f(x+1)$ operation is at the core of the above algorithm for real root isolation (counting).

Univariate Taylor Shift: Parallel Horner's Method

Horner's method

We compute $g(x) = f_0 + (x + 1)(f_1 + \dots + (x + 1)f_d)$ in n steps

$$g^{(0)} = f_d, \ g^{(i)} = (x+1)g^{(i-1)} + f_{d-i} \text{ for } 1 \le i \le d,$$

and obtain $g = g^{(d)}$. One can represent this computation in a Pascal's Triangle.

Given an example $f(x) = a_3 x^3 + a_2 x^2 + a_1 x + a_0$, we have, in Horner's rule as follows.

Thus, $g(x) = f(x + 1) = c_3 x^3 + c_2 x^2 + c_1 x_1 + c_0$. For instance, we can parallelize the addition $a_1 + a_2$, $a_2 + a_3$ and $a_3 + 0$, and so on.

Univariate Taylor Shift: Parallel Divide & Conquer Method

Divide & conquer method

We assume that $d + 1 = 2^{\ell}$ is a power of two. In a precomputation stage, we compute $(1 + x)^{2^{i}}$ for $0 \le i < \ell$. In main stage, with polynomials $f^{(0)}$, $f^{(1)} \in \mathbb{Q}[x]$ of degree less than $\frac{d+1}{2}$, we compute

$$g(x) = f^{(0)}(x+1) + (x+1)^{(d+1)/2} f^{(1)}(x+1),$$

where we compute $f^{(0)}(x+1)$ and $f^{(1)}(x+1)$ recursively.

We parallelize each univariate polynomial multiplication by a DnC method. For example,



Benchmarks (1/2)

Degree	BPAS	CMX-2010	realroot	#Roots
4095	3.31	2.622	7.137	1
8191	13.036	17.11	40.554	1
16383	61.425	124.798	274.706	1
32767	286.46	970.165	2059.147	1
65535	1311.07	7960.57	*Err.	1

Table: Running time of $Bn, d(x) = 2^d x^d + ... + 2^d$ on Intel 12-core

Degree	BPAS	CMX-2010	realroot	#Roots
4095	1.93	1.917	3.941	1
8191	6.467	7.611	29.448	1
16383	25.291	34.198	239.771	1
32767	96.507	172.432	1863.125	1
65535	375.678	995.358	*Err.	1

Table: Running time of Cn, $d(x) = x^d + d$ on Intel 12-core

Benchmarks (2/2)

	Size	BPAS	CMX-2010	realroot	#Roots
Bnd	4096	4.003	5.125	4.955	1
	8192	11.025	25.228	23.754	1
	16384	43.498	127.412	159.245	1
	32768	176.351	609.513	1,011.872	1
	65536	701.682	4,695.31	9,741.249	1
Cnd	4096	0.704	1.209	1.699	1
	8192	1.533	5.228	10.899	1
	16384	5.086	25.296	109.420	1
	32768	18.141	125.902	816.134	1
	65536	66.436	664.438	7,526.428	1
Chebycheff	2048	608.738	594.82	1,378.444	2047
	4096	8,194.06	10,014	35,880.069	4095
Laguerre	2048	1,336.14	1,324.33	3,706.749	2047
	4096	20,727.9	23,605.7	91,668.577	4095
Wilkinson	2048	630.481	614.94	1,031.36	2047
	4096	9,359.25	10,733.3	26,496.979	4095

Table: Running times on AMD 48-core

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www.bpaslib.org