The FFLAS-FFPACK and LinBox libraries

OpenDreamKit Software presentation

Clément Pernet & the LinBox group

September 2, 2015

Matrices can be

Dense: store all coefficients

Sparse: store the non-zero coefficients only

Black-box: no access to the storage, only apply to a vector

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Coefficient domains:

Word size: ▶ integers with a priori bounds

▶ $\mathbb{Z}/p\mathbb{Z}$ for p of ≈ 32 bits

Multi-precision: $\mathbb{Z}/p\mathbb{Z}$ for p of $\approx 100, 200, 1000, 2000, \dots$ bits

Arbitrary precision: \mathbb{Z}, \mathbb{Q}

Polynomials: K[X] for K any of the above

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Requires genericity.

Software stack for exact linear algebra

Arithmetic

GMP, MPIR: multiprecision integers and rationals

YGGOO, NTL: finite fields and polynomials



Software stack for exact linear algebra

Arithmetic

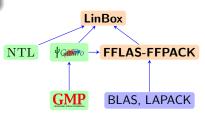
GMP, MPIR: multiprecision integers and rationals

YGGOO, NTL: finite fields and polynomials

BLAS: Basic Linear Algebra
Subroutines (floating point)

FFLAS-FFPACK: Basic Exact Linear Algebra over $\mathbb{Z}/p\mathbb{Z}$,

 $\begin{array}{ll} {\sf LinBox: \ Linear \ Algebra \ over \ } \mathbb{Z}, \mathbb{Z}/p\mathbb{Z} \\ {\sf \ and \ } {\sf \ K}[X] \end{array}$



Software stack for exact linear algebra

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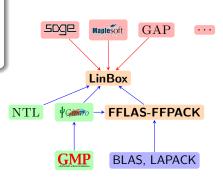
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FFLAS-FFPACK: Basic Exact Linear Algebra over $\mathbb{Z}/p\mathbb{Z}$,

LinBox: Linear Algebra over $\mathbb{Z}, \mathbb{Z}/p\mathbb{Z}$ and K[X]



Outline

- The LinBox library
- 2 Blackbox linear algebra
- 3 Dense linear algebra
- 4 Parallelization

The LinBox project

- International collaboration: Canada, USA, France
- Strongly generic C++ code, focus on efficiency
- ► Free software (LGPL 2.1+)
- $\triangleright \approx 200 \text{ K loc}$
- http://linalg.org/

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Milestones

```
1998 First design: Black box and sparse matrices
```

```
2003 Dense linear algebra using BLAS → FFLAS-FFPACK
```

```
2005 LinBox-1.0
```

2008 Integration in Sage

2012-.. Parallelization

2014 SIMD & Sparse BLAS in FFLAS-FFPACK (Brice's talk)

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- Matrices viewed as linear operators
- ▶ algorithms based on matrix-vector apply only \leadsto cost E(n)



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Structured matrices: Fast apply (e.g. $E(n) = O(n \log n)$)

Sparse matrices: Fast apply and no fill-in

~→

- Iterative methods
- No access to coefficients, trace, no elimination
- ► Matrix multiplication ⇒ Black-box composition

Example: blackbox composition

```
template <class Mat1, class Mat2>
class Compose {
  protected:
    Mat1 _A;
    Mat2 _B:
  public:
    Compose(Mat1& A, Mat2& B) : A(A), B(B) {}
    template < class InVec, class OutVec>
    OutVec& apply (const InVec& x) {
      return _A.apply(_B.apply(x));
```

```
Matrix-Vector Product: building block, \rightsquigarrow costs E(n)
Minimal polynomial: [Wiedemann 86] \rightsquigarrow iterative Krylov/Lanczos methods
```

 $\leadsto O(nE(n) + n^2)$

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Matrix-Vector Product: building block, \rightarrow costs E(n)

Minimal polynomial: [Wiedemann 86] \rightarrow iterative Krylov/Lanczos methods \rightarrow O(nE(n)+n^2)

Rank, Det, Solve: [ Chen& Al. 02] \rightarrow reduces to MinPoly + preconditioners \rightarrow O(nE(n)+n^2)
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Characteristic Poly.: [Dumas P. Saunders 09]

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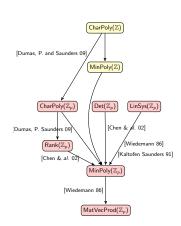
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 $<1969 \!\colon O(n^3)$ for everyone (Gauss, Householder, Danilevskii, etc)

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Matrix Product
                                       O(n^{2.807})
[Strassen 69]:
                                        O(n^{2.52})
[Schönhage 81]
                                       O(n^{2.375})
[Coppersmith, Winograd 90]
                                  O(n^{2.3728639})
  [Le Gall 14]
\rightsquigarrow \mathsf{MM}(n) = O(n^{\omega})
```

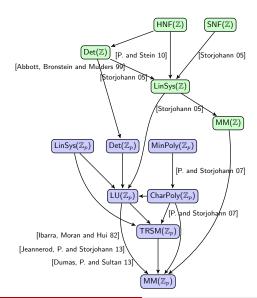
Reductions: linear algebra's arithmetic complexity

< 1969: $O(n^3)$ for everyone (Gauss, Householder, Danilevskii, etc)

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```
Other operations  [Strassen 69]: \qquad Inverse in \ O(n^\omega) \\ [Schönhage 72]: \qquad QR \ in \ O(n^\omega) \\ [Bunch, Hopcroft 74]: \qquad LU \ in \ O(n^\omega) \\ [Ibarra \& al. 82]: \qquad Rank \ in \ O(n^\omega) \\ [Keller-Gehrig 85]: \ CharPoly \ in \\ O(n^\omega \log n)
```

Reductions





Common mistrust

Fast linear algebra is

never faster

numerically unstable

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Lucky coincidence

- ✓ building blocks in theory happen to be the most efficient routines in practice
- → reduction trees are still relevant

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Roadmap

Tune building blocks

(MatMul)

Improve existing reductions

(LU, Echelon)

- ▶ leading constants
- memory footprint

Produce new reduction schemes

(CharPoly)

Ingedients [Dumas, Gautier and P. 02]

ightharpoonup Compute over $\mathbb Z$ and delay modular reductions

$$\rightarrow k \left(\frac{p-1}{2}\right)^2 < 2^{\text{mantissa}}$$

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- ► Cache optimizations

→ numerical BLAS

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$$\,\leadsto\, 9^\ell \left\lfloor \tfrac{k}{2^\ell} \right\rfloor \left(\tfrac{p-1}{2} \right)^2 < 2^{\mathsf{mantissa}}$$

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▶ Strassen-Winograd $6n^{2.807} + \dots$

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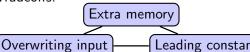
- Fastest integer arithmetic: double, float (SIMD and pipeline)
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with memory efficient schedules [Boyer, Dumas, P. and Zhou 09]

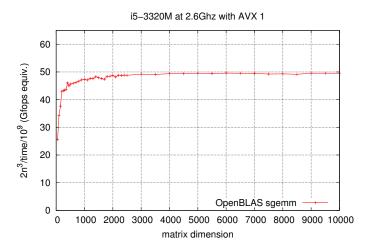
Tradeoffs:

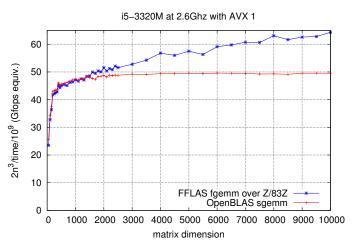


Leading constant

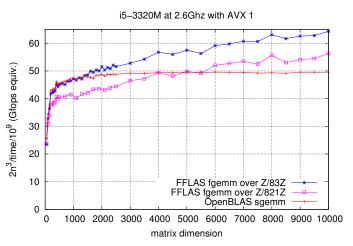
Fully in-place in

 $7.2n^{2.807} + \dots$

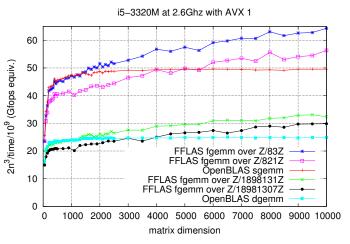




p = 83, $\rightsquigarrow 1 \mod / 10000 \text{ mul.}$



p=83, $\leadsto 1 \mod / 10000$ mul. p=821, $\leadsto 1 \mod / 100$ mul.



 $p = 83, \rightsquigarrow 1 \mod / 10000 \text{ mul.}$ $p = 1898131, \rightsquigarrow 1 \mod / 10000 \text{ mul.}$ $p = 821, \rightsquigarrow 1 \mod / 100 \text{ mul.}$ $p = 18981307, \rightsquigarrow 1 \mod / 100 \text{ mul.}$

Other routines

LU decomposition

▶ Block recursive algorithm \leadsto reduces to MatMul $\leadsto O(n^{\omega})$

n	1000	5000	10000	15000	20000
LAPACK-dgetrf fflas-ffpack	0.024s 0.058s	2.01s 2.46s		48.78s 47.47s	113.66 105.96 s

Intel Haswell E3-1270 3.0Ghz using OpenBLAS-0.2.9

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Characteristic Polynomial

• A new reduction to matrix multiplication in $O(n^{\omega})$.

n	1000	2000	5000	10000
magma-v2.19-9	1.38s	24.28s	332.7s	2497s
fflas-ffpack	0.532s	2.936s	32.71s	219.2 s

Intel Ivy-Bridge i5-3320 2.6Ghz using OpenBLAS-0.2.9

Other routines

LU decomposition

▶ Block recursive algorithm \rightsquigarrow reduces to MatMul \rightsquigarrow $O(n^{\omega})$

n	1000	5000	10000 15000	20000×7.63
•			14.88s 48.78s 16.08s 47.47s	113.66 ×6.59
Intel Haswell E3-12				103.303

Characteristic Polynomial

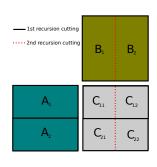
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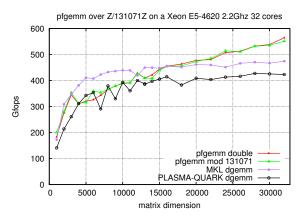
n	1000	2000	5000	10000	×7.5
magma-v2.19-9 fflas-ffpack	1.38s 0.532s		332.7s 32.71 s	2497s × 219.2s	×6.7
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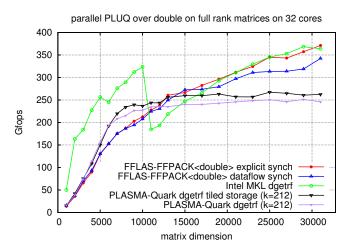
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Parallel matrix multiplication





Gaussian elimination



Thank You.