Workpackage 5:
High Performance Mathematical Computing

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Second OpenDreamKit Project review

Luxembourg, October 30, 2018

High performance mathematical computing

Mathematical computing

Computing with a large variety of objects

- $\mathbb{Z}, \mathbb{Q}, \mathbb{Z}/p\mathbb{Z}, \mathbb{F}_q,$ $175417188143890121646 32$

for applications where all digits matter.

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- Polynomials over $\mathbb{Z}, \mathbb{Q}, \mathbb{Z}/p\mathbb{Z}, \mathbb{F}_q,$ $\qquad \frac{2}{5}x^3 + x^2 - \frac{1}{19}x + 2$

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- Matrices of polynomials over $\mathbb{Z}, \mathbb{Q}, \mathbb{Z}/p\mathbb{Z}, \mathbb{F}_q$, $\quad \begin{bmatrix} 3x^2+3 & 2x^2+3 \\ 4x^2+1 & x^2+4x+4 \end{bmatrix}$

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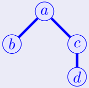
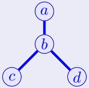
- Tree algebra

$\frac{3q^2-q^5}{q^5+2q^4+3q^3+3q^2+2q+1}$ 

$+ \frac{2q}{q^4+q^3+2q^2+q+1}$ 

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Need for High performance: applications where size matters:

Experimental maths: testing conjectures

- larger instances give higher confidence

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Algebraic cryptanalysis: security = computational difficulty

- key size determined by the largest solvable problem

Example

Breaking RSA by integer factorization: $n = pq$. Last record:

- n of 768 bits
- linear algebra in dimension $192\,796\,550$ over $\mathbb{F}_2$ (105Gb)
- About 2000 CPU years

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3D data analysis, shape recognition:

- via persistent homology
- large sparse matrices over $\mathbb{F}_2$, $\mathbb{Z}$

Goal: delivering high performance to maths users

Systems : GAP, PARI/GP, SageMath, Singular

Components : FLINT, MPIR, LinBox, PPL, NumPy

Goal: delivering high performance to maths users

Harnessing modern hardware $\rightsquigarrow$ parallelisation

- in-core parallelism (SIMD vectorisation)
- multi-core parallelism
- distributed computing: clusters, cloud

Systems : GAP, PARI/GP, SageMath, Singular

Components : FLINT, MPIR, LinBox, PPL, NumPy

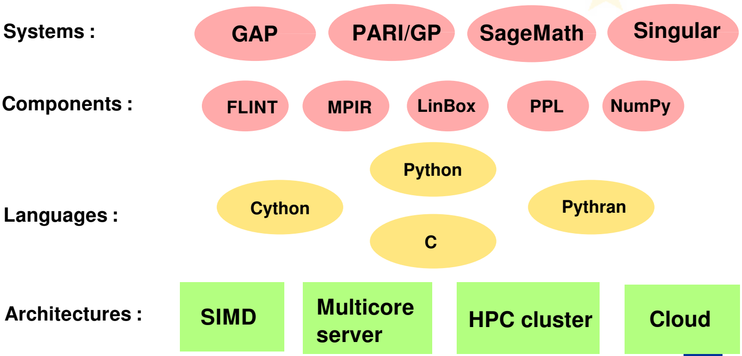
Architectures : SIMD, Multicore server, HPC cluster, Cloud

Goal: delivering high performance to maths users

Languages

- Computational Maths software uses high level languages (e.g. Python)
- High performance delivered by languages close to the metal (C, assembly)

$\rightsquigarrow$ compilation, automated optimisation



High performance mathematical computing

Goal:

- Improve/Develop parallelization of software components
- Expose them through the software stack
- Offer High Performance Computing to VRE's users

Milestone M8: Seamless use of parallel computing architecture in the VRE (proof of concept)

Astrid wants to run compute intensive routines involving both dense linear algebra and combinatorics. She has access through a JupyterHub-based VRE to a high end multi-core machine which includes a vanilla SAGE installation. She automatically benefits from the HPC features of the underlying specialized libraries (LinBox, ...). This is a proof of concept of the overall framework to integrate the HPC advances of specialized libraries into a general purpose VRE. It will prepare the final integration of a broader set of such parallel features for the end of the project

Outline

Workpackage management

Exact linear algebra

- Exact linear algebra algorithms and implementations (D5.12).
- Distributed computing

Combinatorics

- Refactor and optimize Sage's Combinatorics (D5.11)

Progress report on other tasks

- T5.1: Pari
- T5.2: GAP
- T5.4: Singular

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Outcome of WorkPackage 5

Component	Review 1	Review 2	Final review
T5.1 Pari/GP			D5.16
T5.2 GAP			D5.15
T5.3 LinBox		D5.12	D5.14
T5.4 Singular	D5.6, D5.7		D5.13
T5.5 MPIR	D5.5, D5.7		
T5.6 Combinatorics	D5.1	D5.11	
T5.7 Pythran	D5.2	D5.11	
T5.8 SunGrid Engine	D5.3		

Overall

- over 20 software relases were cut
- 7 research papers

Addressing recommendations of review 1

Recommendation 10: *Regarding WP5,* **make contacts** *with HPC community in order to ascertain current state-of-the-art. The work in this WP needs to be* **nearer the leading edge***.*

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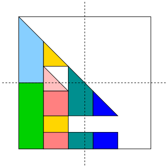
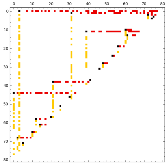
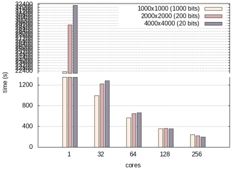
Leading edge achievements in linear algebra

- symmetric factorization outperforms LAPACK implementation
- new non-hierarchical generator for quasiseparable matrices
- large scale parallelization of rational linear solver







Strengthening interactions with numerical HPC community

Existing connection

Dense linear algebra numerical BLAS used for exact FFLAS for 17 years

Pointwise interactions: J. Dongarra, L. Grigori, J-Y. L'Excellent, etc

Publications to in main HPC venues: SIAM-PPSC, EuroPar, PMAA, ParCo

Animation: involved in the French CNRS *Calcul* working group (Sci. Comp.)

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Recently established

- With the `BLIS` group:
  - Reporting bugs (SIMD vectorization)
  - Sharing experience in implementing Strassen's algorithm
- On-going collaboration with T. Mary (`Mumps`) and S. Chandrasekaran (UCSB) on quasiseparable matrix algorithmic

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Task 5.3: LinBox, High performance exact linear algebra

Mathematics is the art of reducing any problem to linear algebra

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Linear algebra: a key building block for HPC

Similarities with numerical HPC

- central elementary problem to which others reduce to
- (rather) simple algorithmic
- high compute/memory intensity

Task 5.3: LinBox, High performance exact linear algebra

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Linear algebra: a key building block for HPC

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Specificities

- Multiprecision arithmetic $\Rightarrow$ lifting from finite precision ($\mathbb{F}_p$)
- Rank deficiency $\Rightarrow$ unbalanced dynamic blocking
- Early adopter of subcubic matrix arithemtic $\Rightarrow$ recursion

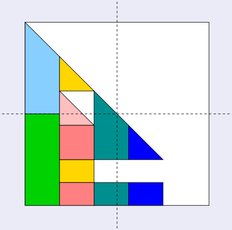
D5.12: Exact linear algebra algorithms and implementations. Library maintenance and close integration in mathematical software for LinBox library

1. Algorithmic innovations:
   1.1 Rank deficient dense Gaussian elimination
   1.2 Quasiseparable matrices
   1.3 Outsourced computing security
2. Software releases and integration:
   2.1 LinBox ecosystem: `LinBox`, `fflas-ffpack`, `givaro`
   2.2 `SageMath` integration

Rank deficient dense Gaussian elimination

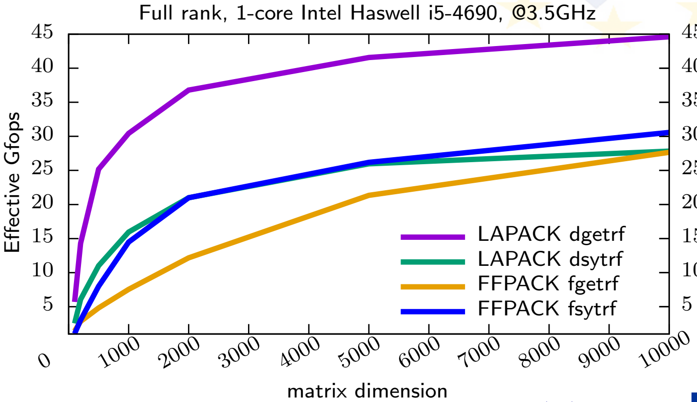
[ISSAC'18] Symmetric triangular factorization

- First unconditional recursive algorithm
- Pivoting revealing the Rank Profile Matrix
- $O(n^2 r^{\omega-2})$ ($= 1/3n^3$ with $\omega = 3, r = n$)
- Also hot topic in numerical linalg
  (LAPACK Working notes 294, Dec'17)



LAPACK vs FFPACK modulo 8 388 593

	LAPACK		FFPACK	
n	dgetrf (LU)	dsytrf (LDLT)	fgetrf (LU)	fsytrf (LDLT)
5000	2.01s	1.60s	3.90s	1.59s
10000	14.95s	11.98s	24.12s	10.90s

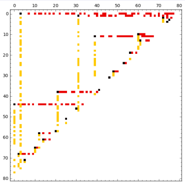


Quasiseparable matrices

Matrices with low off-diagonal rank

[ISSAC'16, JSC'18] New compact representation and algorithms

- Matches the best space complexities
- Reduction to matrix multiplication
- **Breakthrough:** Flat representation (non hierarchical)



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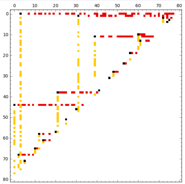

Follow-up: on-going collaboration with numerical HPC experts:

- S. Chandrasekaran (UCSB)
- T. Mary (U. Manchester, `Mumps`)

Software releases and integration

LinBox ecosystem

`givaro`: field/ring arithmetic

`fflas-ffpack`: dense linear algebra over finite field

`LinBox`: exact linear algebra

Tightly integrated in `SageMath`

Software releases and integration

LinBox ecosystem

givaro: field/ring arithmetic	4 releases
fflas-ffpack: dense linear algebra over finite field	6 releases
LinBox: exact linear algebra	6 releases
Tightly integrated in SageMath	13 tickets

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`givaro`: field/ring arithmetic	4 releases
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Featuring

- Full functional implementations of new algorithmic contributions
- Improved vectorization and parallel routines
- Drastic improvement of reliability (continuous integration, test-suite coverage, randomized certificates, etc)

Distributed computing (on-going work)

D5.14: Distributed exact linear system solving

- 2 full time engineers
- Communication and serialization layer done
- Prototype MPI parallelization of Chinese remainder based solver.

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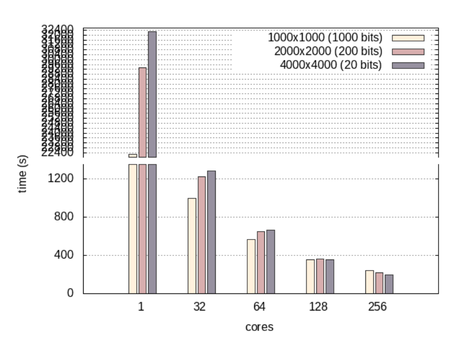
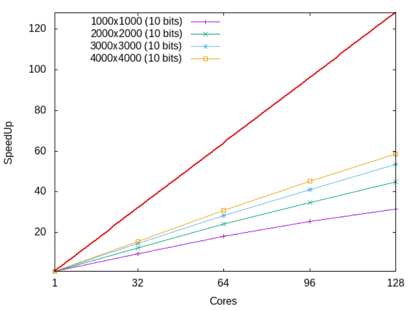


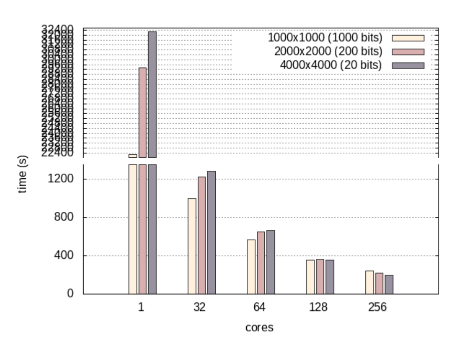


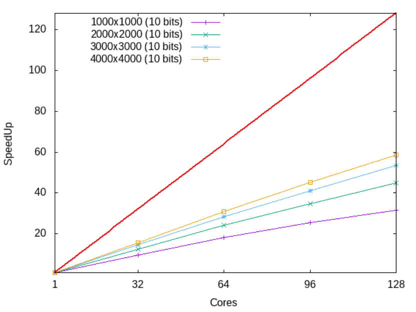
Distributed computing (on-going work)

D5.14: Distributed exact linear system solving

Roadmap:

- Major refactorization of LinBox solver code under way
- Parallelization of Dixon-lifting solver
- Hybrid combination of CRT+Dixon.
- Hyrbid OpenMP-MPI implementation





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Task 5.6: HPC infrastructure for Combinatorics

Parallel algebraic computations exhibit high degrees of irregularity, at multiple levels and make no use of floating-point operations. This combination means that symbolic computations are not suited to conventional HPC paradigms.
– P. Maier, D. Livesey, H.-W. Loidl, P. Trinder

General situation

Given a set S of combinatorial objects we want to

- find (or pick at random) an element of S
- list (or count) the elements of S

Specificities of combinatorics

- **huge**: S does not fit in memory
- **embarassingly parallel**: $S = S_1 \cup \ldots \cup S_k$
- **unbalanced**: S_i sizes are highly unbalanced

D5.11: Refactor and optimise the existing combinatorics Sage code using the new developed Pythran and Cython features.

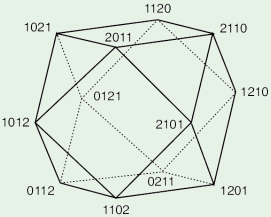
Algorithmic innovations and software integration through examples:

1. Example 1: polytopes
2. Example 2: numerical semigroups

Example 1: polytopes (description)

Example

Some combinatorial objects can be encoded as integer vectors in polytopes.



- Efficient algorithms available (*e.g.* Double Description, Barvinok)
- High performance libraries (*e.g.* `PPL`, `Normaliz`, `Polymake`)
- Useful for many combinatorial problems

Example 1: polytopes (ODK work)

ODK outcomes

`pplpy` library: Python interface to the high performance Parma Polyhedra Library (rational polytopes)

`e-antic` library: C/C++ library for computations over embedded number fields. Building block for multithread polytope computations in Normaliz over number fields.

Workshop: Sage Days 84

`SageMath`: improvement of native code and libraries interfaces

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ODK outcomes

`pplpy` library: Python interface to the high performance Parma Polyhedra Library (rational polytopes) — 6 releases

`e-antic` library: C/C++ library for computations over embedded number fields. Building block for multithread polytope computations in Normaliz over number fields. — release planned

Workshop: Sage Days 84

`SageMath`: improvement of native code and libraries interfaces — 10 tickets

Example 2: semigroups (description)

Example

Numerical semigroup are certain subsets of non-negative integers.

$$\langle 1 \rangle$$
$$\langle 2,3 \rangle$$
$$\langle 2,5 \rangle \qquad \langle 3,4,5 \rangle$$
$$\langle 2,7 \rangle \quad \langle 3,4 \rangle \quad \langle 3,5,7 \rangle \quad \langle 4,5,6,7 \rangle$$
$$\vdots \qquad \vdots \qquad \vdots \qquad \vdots$$

- Many mathematical open mathematical questions
- Highly unbalanced tree

Example 2: semigroups (ODK work)

A SageMath implementation of work-stealing map-reduce

- Work stealing algorithm (Leiserson-Blumofe)
- Easy to use, easy to call from SageMath with many use cases
- Scale well with the number of CPU cores and reasonably efficient (given that it is Python code).

A typical speedup (parallelization of binary sequences)

# processors	1	2	4	8
Speedup	$\times 1$	$\times 1.55$	$\times 2.43$	$\times 2.87$

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integrated in SageMath

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HPCombi: an experimental C++ library

- innovative SIMD code for combinatorics
- fine grained parallelization using Intel Cilk technology
- already in use for mathematical projects (numerical semigroups)

Operation	Speedup
Sum of a vector of bytes	$\times 3.81$
Sorting a vector of bytes	$\times 21.3$
Inverting a permutation	$\times 1.97$
Number of cycles of a permutation	$\times 41.5$
Number of inversions of a permutation	$\times 9.39$
Cycle type of a permutation	$\times 8.94$

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Open-source library

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T5.1: Pari

D5.16: Pari Suite release, fully supporting parallelization

- D5.10 (merged in D5.16):
  Generic parallelization engine is now mature (released since nov.2016).
  Support POSIX-threads and MPI.
- Current work: applying it throughout the library
  - Chinese remaindering
  - Rational linear algebra
  - Discrete logarithm
  - Resultants
  - APRCL primality testing

T5.2: GAP

D5.15: Final report of GAP development

- 8 releases were cut integrating contributions of D3.11 and D5.15
- Towards an integration of HPC-GAP: main release GAP-4.9
  - Build system refactoring
  - Ability to compile in HPC-GAP compatibility mode
- Work in progress:
  - Multithreaded linear algebra: at the level of the `Meataxe` library
  - Introspection functionalities: on-the-fly optimisation decision

T5.4 Singular

D5.13: Parallel sparse polynomial multiplication

`FLINT` now supports fast sparse multivariate polynomials:

- addition, subtraction, multiplication,
- division, division with remainder, GCD
- evaluation (and partial evaluation), composition

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Parallelization of the (sparse) multiplication

threads	time (ms)	speedup
1	148661	x1.0
2	76881	x1.9
3	54798	x2.7
4	42855	x3.4
5	37017	x4.0
6	30892	x4.8
7	28365	x5.2
8	28048	x5.3

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- Planned improvements to the memory manager $\Rightarrow$ closer to linear scaling
- Parallel division and GCD implementations are in progress.
- Integration into Factory/Singular remains to be done

Conclusion

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Overall

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- 7 research papers

Backup Slides

Outsourced computing security (D5.12)

Exploratory aspect: Computation over the Cloud

Outsourcing computation on the cloud:

- trusted lightweight client computer
- untrusted powerful cloud server

$\Rightarrow$ need for certification protocols

Multiparty computation:

- each player contribute with a share of the input
- shares must remain private

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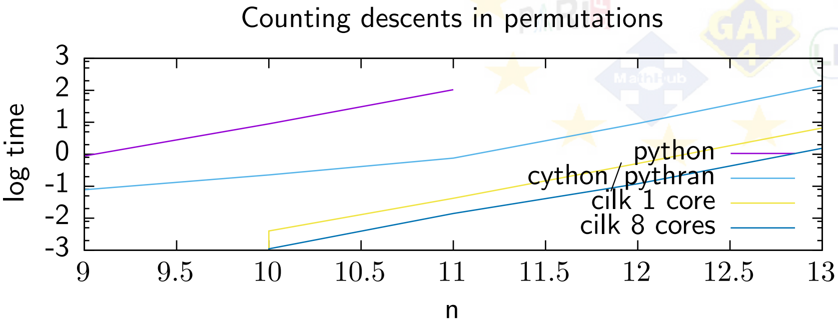
Contribution

ISSAC'17: Linear time certificates for LU, Det., Rank Profile matrix, etc

In submission: Secure multiparty Strassen's algorithm

Exploration: Python, Cython, Pythran and Cilk (D5.8)

workshop: Interfacing (math) software with low level libraries



- Python (interpreted language) slow.
- Cython/Pythran (Python to C compilers) efficient.
- Cilk (SIMD and multithread parallelism) very promising.