Workpackage 5:
High Performance Mathematical Computing

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Final OpenDreamKit Project review

Luxembourg, October 30, 2019

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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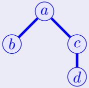
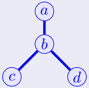
- Tree algebras

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

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

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High performance mathematical computing

Need for High performance: applications where size is crucial:

Experimental maths: testing conjectures

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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

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Harnessing modern hardware ⇝ 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

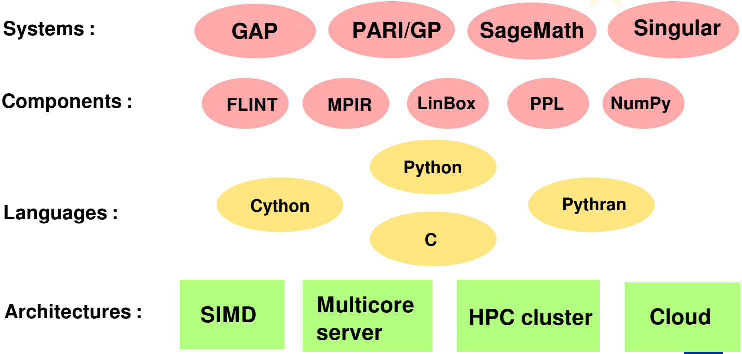
Architectures : SIMD · Multicore server · HPC cluster · Cloud

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

Outcome of WorkPackage 5

Component	Review 1	Review 2	Final review
T5.1 Pari/GP			D5.16
T5.2 GAP			D5.15
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Overall

- 31 software releases
- 16 research papers

Outline

Context and Focus

T5.1: Number theory with PARI/GP

T5.2: Group theory with GAP

T5.3: Exact linear algebra with LinBox

T5.4: Polynomial arithmetic with Singular

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Computational Kernels: linear algebra

Mathematics is the art of reducing any problem to linear algebra

– W. Stein

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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

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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

Computational kernels: arithmetic

- Wide variety of computing domains: $\mathbb{Z}, \mathbb{Q}, \mathbb{Z}/p\mathbb{Z}, \mathbb{F}_q, \mathbb{F}_q[X], \mathbb{Z}[X, Y, Z], ..$
- possibly with dynamic size

Challenge

- most often memory intensive operations ➔ hard to parallelize
- very fine grain, but billions of instance ➔ fine tuning

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PARI-GP

PARI ecosystem

PARI library: dedicated routines for number theory

PARI-GP: an interactive system

GP2C: a GP to C compiler

Generic parallelization engine for the whole suite

Delivers support for

- sequential computations
- POSIX threads
- MPI for distributed computing

Features:

- Same code base
- automated parallelization
- full control for power users/developpers

Main Achievements

- Fast linear algebra over the rationals and cyclotomic fields
- Fast Chinese remainders and multimodular reduction
- Parallel polynomial resultant
- Fast modular polynomials and applications
- MPQS integer factorization rewrite

Well-honed strategy after preliminary assessment

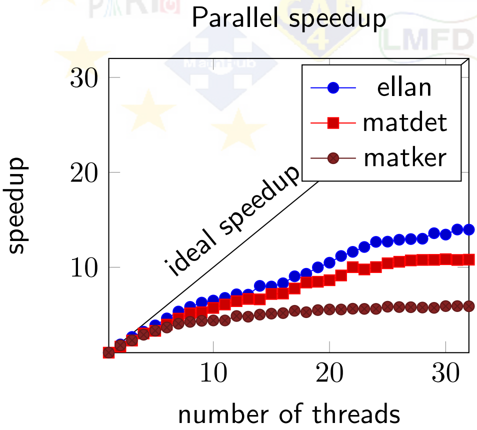
- Creation of "worker" functions from existing code
- Insertion of actual parallel instructions
- Incremental buildup, independently instrumenting one high-level function at a time.

Highlight

Linear algebra over rationals:

- Required for cyclotomic rings (Allombert, 2016-17)
- Fast Chinese remaindering (Allombert, 2017)
- Fast CUP decomposition over finite fields (Bruin, 2018)
- Parallelization (Allombert, Belabas, 2017-19)

Fourier transform of L-functions



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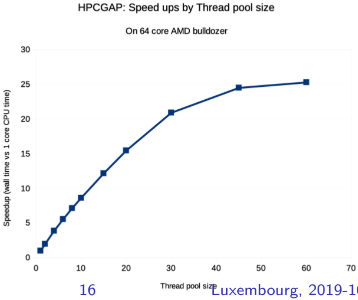
HPC GAP

HPC-GAP

- Multi-threaded GAP.
- Targets:
  - multicore servers.
  - good speedups
  - high level abstraction

Achievement

- Fork from GAP, diverged for a long time
- Huge effort to bring it back in:
  GAP 4.9.1 (Month 33).
  → first GAP release with HPCGAP integrated as a compile-time option



Dense linear algebra over small finite fields

- Matrix multiplication, Gaussian elimination, echelon forms, etc
- A key kernel for many GAP computations

MeatAxe64

A new C and assembler library, tuned for performance at all levels:

- new data representations and assembler kernels
- new algorithms for many fields
- control of cache usage and memory bandwidth
  → allowing for sharing between threads and cores
- purpose built highly efficient task farm
  → 1M x 1M dense matrix multiply over GF(2) in 8 hours (64 core AMD bulldozer).

Fully available from GAP.

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Parallel Rational solver algorithmic

Method	Bit complexity
Gauss over $\mathbb{Q}$	$2^{O(n)}$
Gauss $\mod$ bound(sol)	$O(n^5)$
Chinese Remaindering	$O\tilde{}(n^4)$
p-adic lifting	$O\tilde{}(n^3)$

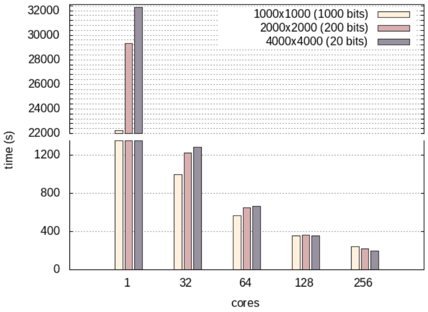
Chinese Remainder

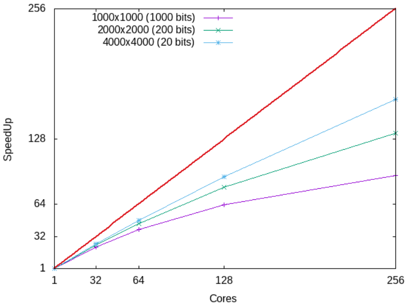
1. Solve the system independently modulo $p_1, p_2, \ldots, p_k$
2. Reconstruct a solution modulo $p_1 \times p_2 \times \ldots, p_k$.
3. Reconstruct over $\mathbb{Q}$

p-adic lifting

1. Solve the system modulo p
2. Iteratively lift the solution modulo $p^2, p^3, \ldots, p^k$
3. Reconstruct over $\mathbb{Q}$

Distributed memory Chinese Remaindering





Conclusions

- (almost) embarrassingly parallel
- but overwhelming computational cost ($O\tilde{}(n^4)$)
- hybrid OpenMP-MPI version slightly slower but better memory efficiency

Shared memory p-adic lifting

A new hybrid algorithm: Chinese Remaindering within p-adic lifting

- Smaller critical path
- Higher degree of parallelism

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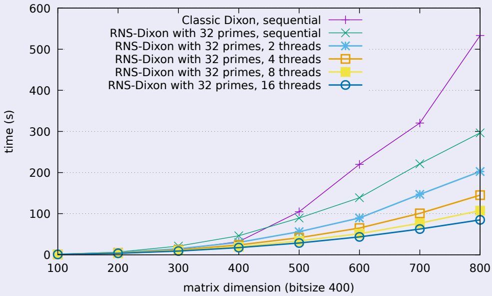
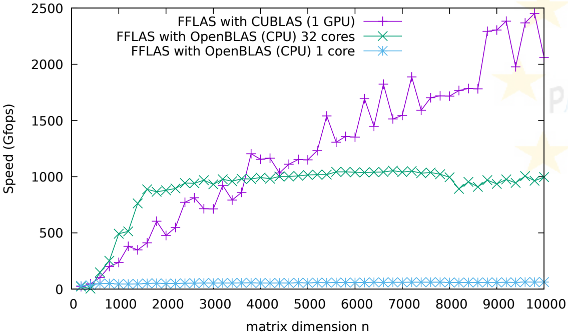
Improving state of the art efficiency

- Improved sequential efficiency (improved memory access pattern, BLAS3)
- Chinese remaindering delivers good parallel scaling



GPU enabled `fflas-ffpack`



- Matrix product over $\mathbb{Z}/131071\mathbb{Z}$
- 32 Skylake-X cores (AVX512)
- 1 Nvidia Tesla V100 GPU

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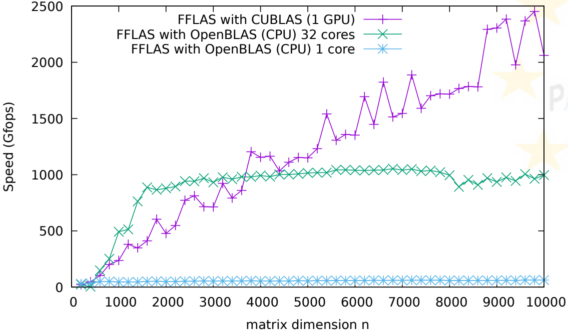

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Limitations and perspectives

Bottleneck in the transfer between GPU and RAM

- deport more computations to the GPU → dedicated GPU kernels
- communication avoiding block scheduling → deep structural change

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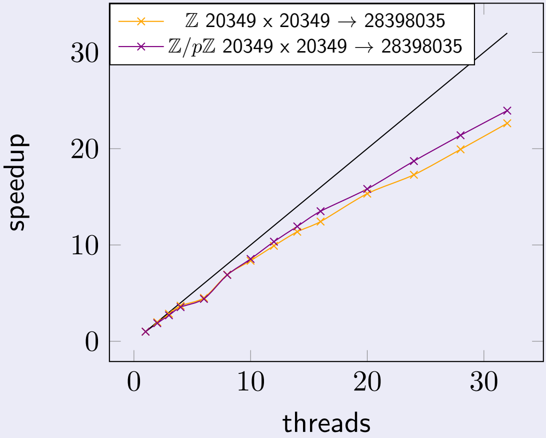
Main achievements

Multivariate Polynomial Multiplication in `FLINT`



- over $\mathbb{Z}$, $\mathbb{Q}$, $\mathbb{F}_p$, $\mathbb{F}_{p^n}$ for $p < 2^{64}$.
- Lex, degLex and degGrevLex ordering supported
- Sequential alg: improves `Singular`'s
- Close to linear scaling
- `Singular` now relies on `FLINT`

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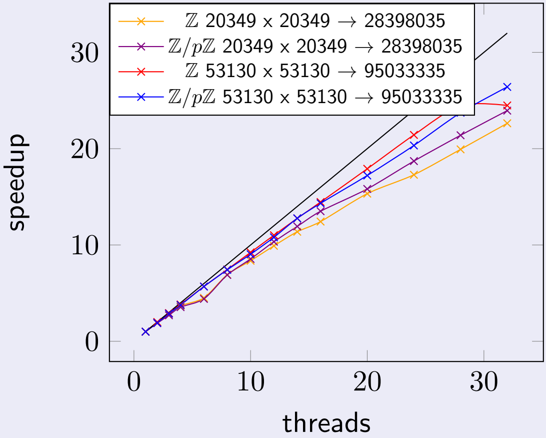

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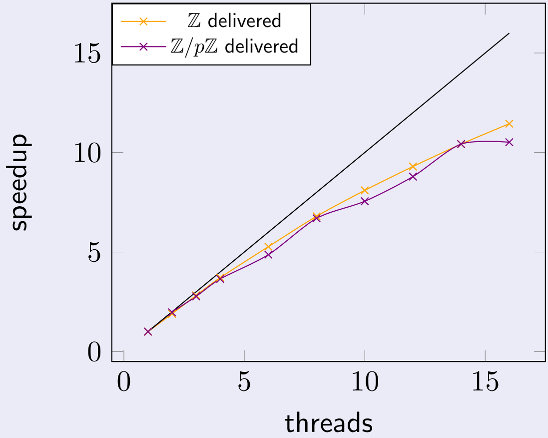

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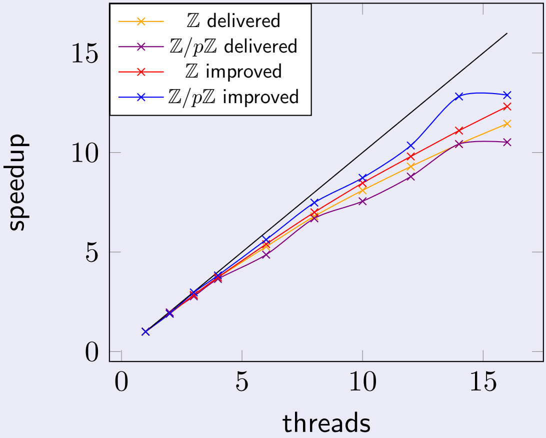

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- Causes performances fickle
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New directions

Application driven:

- More orderings: block, weighted
- Factorization: (harnessing most T5.4 contributions)

Conclusion

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Lessons learnt

From dedicated to general purpose HPC components:

- Early instances of HPC computer algebra: dedicated to some target application (breaking RSA, etc)
- Building a general purpose HPC component:
  - challenging
  - longer term sustainability

Identifying the right place to focus efforts on

- Premature focus on embarassingly parallel distributed computing
- Might as well improve a more difficult algorithm on multicore servers

Risk of technology dependency

- Cilk: from success to shut-down
- Interchangeability and modularity (PARI, LinBox)

Perspectives

Deployment of architecture dependent software stacks

- dynamic runtime configuration
  - ➔ user decision based on algorithms (high level), not systems (low level)
  - ➔ compilation hurdle, vs slick interface of the VRE
- extend high level control over parallel resources: GPUs, cluster nodes, etc
- keep as much HPC features as possible in virtualization images