What can you do *exactly*, with fast floating point linear algebra

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Sage Seminar
January 24, 2007

Outline

1. Numerical linear algebra: the BLAS
   - Why ?
   - BLAS
   - Optimizations
2. FFLAS: a BLAS for finite fields
   - Delayed reductions
   - Cache tuning
   - Sub-cubic algorithm
   - Memory efficiency
3. Over the integers
4. Perspectives
   - Dedicated BLAS
   - High precision approximate computations

Why ?

Huge range of applications in numerical computations

- All PDE based computations: Wheather forecasts, mechanical designs, computational chemistry, ...
- ODE, Control, ...

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⇒design for long term optimizations and portability ?

BLAS : Basic Linear Algebra Subroutines

1979 [Lawson & Al.], first set of Fortran subroutines

1988 [Dongarra & Al], level 2 (MatVect)

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Optimized implementations :

- machine specific by computer vendors (Intel, SGI, IBM, ...)
- architecture independent: ATLAS, GOTO.

Features

4 data types : float (s), double (d), complex (c), double cpx (z)

3 levels :

- level 1 Vector ops (rotation, dot-prod, add, scal axpy,...)
- level 2 Matrix-Vector ops (MatVect prod, triangular system solve, tensor product,...)
- level 3 Matrix-Matrix ops (MatMul, multi triangular system solve,...)

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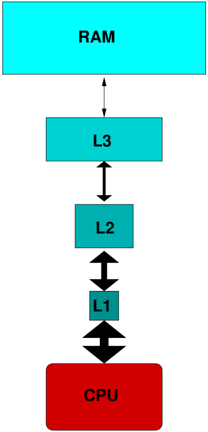
Optimizing data locality

Memory considerations:

- CPU-Memory communication: bandwidth gap
  ⇒Hierarchy of several cache memory levels



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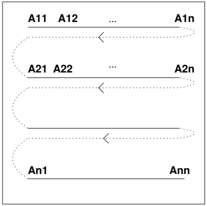

Optimizing data locality

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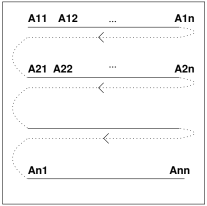
- CPU-Memory communication: bandwidth gap
  ⇒Hierarchy of several cache memory levels
- Row major representation of matrices
- a RAM memory access can fetch a bunch of contiguous elements



Optimizing data locality

Comparing

for i=1 to n **do**
  for j=1 to n **do**
    for k=1 to n **do**
      $C_{i,j} \leftarrow C_{i,j} + A_{i,k}B_{k,j}$
    end for
  end for
end for

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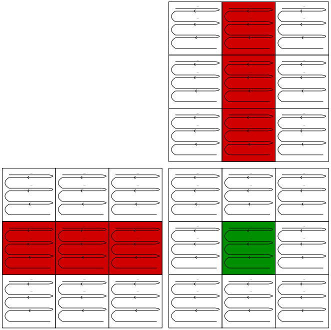
Further memory optimizations

Larger dimensions: cache blocking.
⇒split matrices into blocks, s.t. their product can be computed within the cache.



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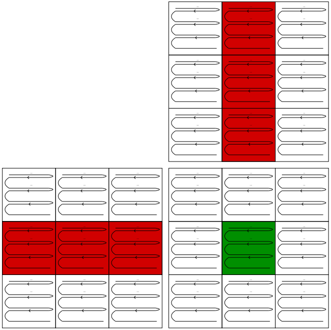

Reuse of the data

- if `Work` $\gg$ `Data` : memory fetch is amortized
  ⇒reach the peak performance of the CPU
- Matrix multiplication: $n^3 \gg n^2$
  ⇒well suited for block design

Arithmetic optimizations

- fma (fused multiply and accumulate) $z \leftarrow z + x * y$
- pipeline
- SSE
- ...

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Tends to give advantage to floating point arithmetic up to now.

Outline

Overview

- word sized finite fields : elements can be represented on 16, 23, 32, 53 or 64 bits
- Delayed modular reductions : avoid unnecessary field arithmetic by computing over $\mathbb{Z}$ as much as possible.
- Cache tuning
- Fast sub-cubic algorithm

Delayed reductions

Existence of 2 ring homomorphisms :

- $\Phi : GF(q) \rightarrow \mathbb{Z}$
- $\Psi : \mathbb{Z} \rightarrow GF(q)$

$$\text{s.t.} \quad \begin{array}{ccc} GF(q) & \xrightarrow{\Phi} & \mathbb{Z} \\ \downarrow +_{GF(q)}, \times_{GF(q)} & & \downarrow +_{\mathbb{Z}}, \times_{\mathbb{Z}} \\ GF(q) & \xleftarrow{\Psi} & \mathbb{Z} \end{array} \quad \text{commutes}$$

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commutes

$\mathbb{Z}_p$: $\Phi = Id, \Psi : x \to x \mod p$

$GF(p^k)$: $\Phi : P(X) \to P(\gamma)$ with $\gamma > nk(p-1)$. (γ-adic reconstruction).

Delayed reductions

⇒compute over $\mathbb{Z}$ with word size elements (int, long, float double)
⇒perform the necessary back conversion (Ψ) only when necessary.
Conditions of validity :

$$\mathbb{Z}_p : \; n(p-1) < 2^m$$
$$GF(p^k) : \; q^(2k-1) < 2^m \text{ and } \gamma > nk(p-1).$$

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Cache tuning

Could mimic the numerical BLAS.
$\Rightarrow$huge amount of work
Instead :

Reuse the existing technology: compute with floating points and use BLAS.

Pros:

- floating point arithmetic is better optimized
- long term efficiency: rely on the numerical community

Cons:

- exponent is useless
- integer arithmetic may become as efficient

Strassen-Winograd algorithm

$$\begin{bmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix},$$

- 8 additions:

$$\begin{array}{ll} S_1 \leftarrow A_{21} + A_{22} & T_1 \leftarrow B_{12} - B_{11} \\ S_2 \leftarrow S_1 - A_{11} & T_2 \leftarrow B_{22} - T_1 \\ S_3 \leftarrow A_{11} - A_{21} & T_3 \leftarrow B_{22} - B_{12} \\ S_4 \leftarrow A_{12} - S_2 & T_4 \leftarrow T_2 - B_{21} \end{array}$$

- 7 recursive multiplications:

$$\begin{array}{ll} P_1 \leftarrow A_{11} \times B_{11} & P_5 \leftarrow S_1 \times T_1 \\ P_2 \leftarrow A_{12} \times B_{21} & P_6 \leftarrow S_2 \times T_2 \\ P_3 \leftarrow S_4 \times B_{22} & P_7 \leftarrow S_3 \times T_3 \\ P_4 \leftarrow A_{22} \times T_4 & \end{array}$$

- 7 final additions:

$$\begin{array}{ll} U_1 \leftarrow P_1 + P_2 & U_5 \leftarrow U_4 + P_3 \\ U_2 \leftarrow P_1 + P_6 & U_6 \leftarrow U_3 - P_4 \\ U_3 \leftarrow U_2 + P_7 & U_7 \leftarrow U_3 + P_5 \\ U_4 \leftarrow U_2 + P_5 & \end{array}$$

- The result is the matrix: $C = \begin{bmatrix} U1 & U5 \\ U6 & U7 \end{bmatrix}$

Strassen-Winograd algorithm

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Over finite fields : not problem

- update the validity condition for delayed reductions from

$$k(p-1)^2 < 2^{53}$$

to

$$\left(\frac{1+3^l}{2}\right)^2 \left\lceil \frac{k}{2^l} \right\rceil (p-1)^2 < 2^{53}$$ for l recursive levels.

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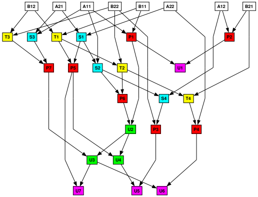
- temporary memory allocations

Memory requirements of Winograd's algorithm



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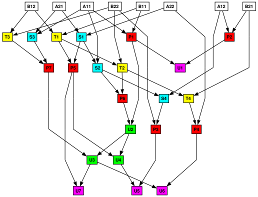

- $C \leftarrow A \times B + C$ $\Rightarrow$from 3 to 2 temp. (3 pre-adds)
- $C \leftarrow A \times B + C$ $\Rightarrow$from 3 to 2 temp. (2 pre-adds, overwriting inputs)
- $C \leftarrow A \times B$ fully in-place (overwriting inputs)

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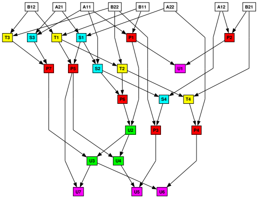

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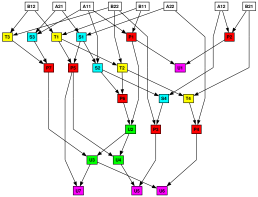

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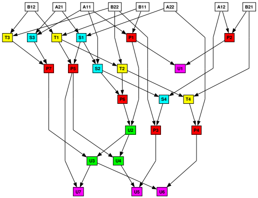

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$\Rightarrow$yes $7.2n^{2.807}$ instead of $6n^{2.807}$

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$\mathbb{Z}_5$	1	4	4
$\mathbb{Z}_7$	6	4	3

$$24 = 4 \cdot 5 \cdot 5^{-1[7]} + 3 \cdot 7 \cdot 7^{-1[5]}$$

Valid, if $5 \times 7 \geq 24$

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MatMul : $\prod_i p_i \geq n(p-1)^2$

$\Rightarrow \log_{2^m} n + 2 \leq 3$ primes

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Dedicated exact BLAS

Exact computations:

- new SSE standard will include integer pipeline
  $\Rightarrow$get rid of floating point arithmetic
- specialized BLAS over GF(2)
  - compact storage
  - method of 4 russians
  - ...
- Top layer for integer BLAS (using CRT, lifting, and multiprecision GMP/MPIR)

High precision approximate computations

multiprecision floating point: no fixed sized arithmetic

- no efficient cache tuning possible

multiprecision integers/rational: finite fields arithmetic available through CRT and lifting

- cache tuning possible
- but higher complexity

$\Rightarrow$hybrid approaches (bounded height good rational approximations) .

Thank You