Multi-precision computations & high performance

A delicate marriage

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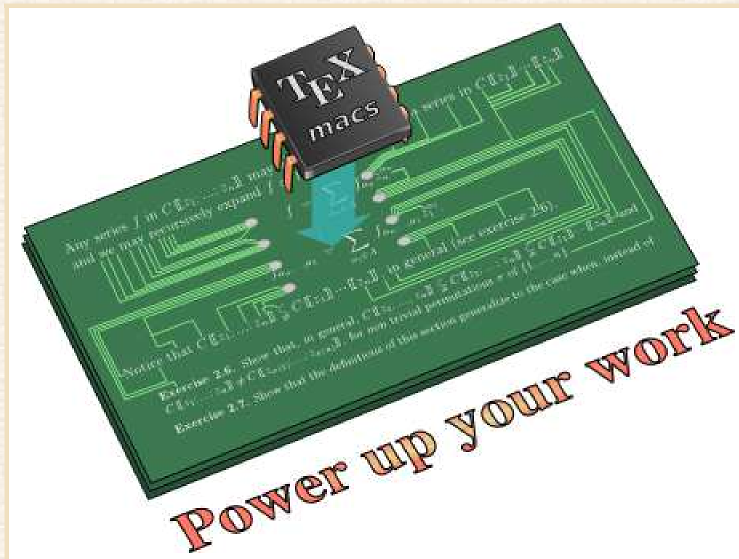

Bangalore, 2011

http://www.TEXMACS.org

The silly remark not to make

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"Why not perform all computations using 8 bits of precision?"

When do we need multiple precision arithmetic?

Large condition numbers

Condition number $\kappa \geqslant 2^{52}$ implies double precision arithmetic makes no sense

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Example: Inversion of a matrix M with

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Example: integration of a dynamical system $Y' = \Phi(Y), Y(0) = C$ near a singularity σ

$$\kappa\left(\frac{\partial Y(\sigma - \varepsilon)}{\partial C}\right) \geqslant 2^{52}$$

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Classical: pick precision p with $\kappa\, 2^{-p} \leqslant \varepsilon$, that is $p \geqslant \phi(p_\varepsilon) = p_\varepsilon + \log_2 \kappa$ with $p_\varepsilon = \log_2 \frac{1}{\varepsilon}$

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Asymptotic extrapolation for a favourable sequence f_n with

$$f_n \approx \alpha^n \left(\frac{a_0 \log n + b_0}{n^0} + \frac{a_1 \log n + b_1}{n^1} + \frac{a_2 \log n + b_2}{n^2} + \cdots \right)$$

Problem: cost to determine α with relative error $\varepsilon > 0$?

Compute $f_0, \ldots, f_N$

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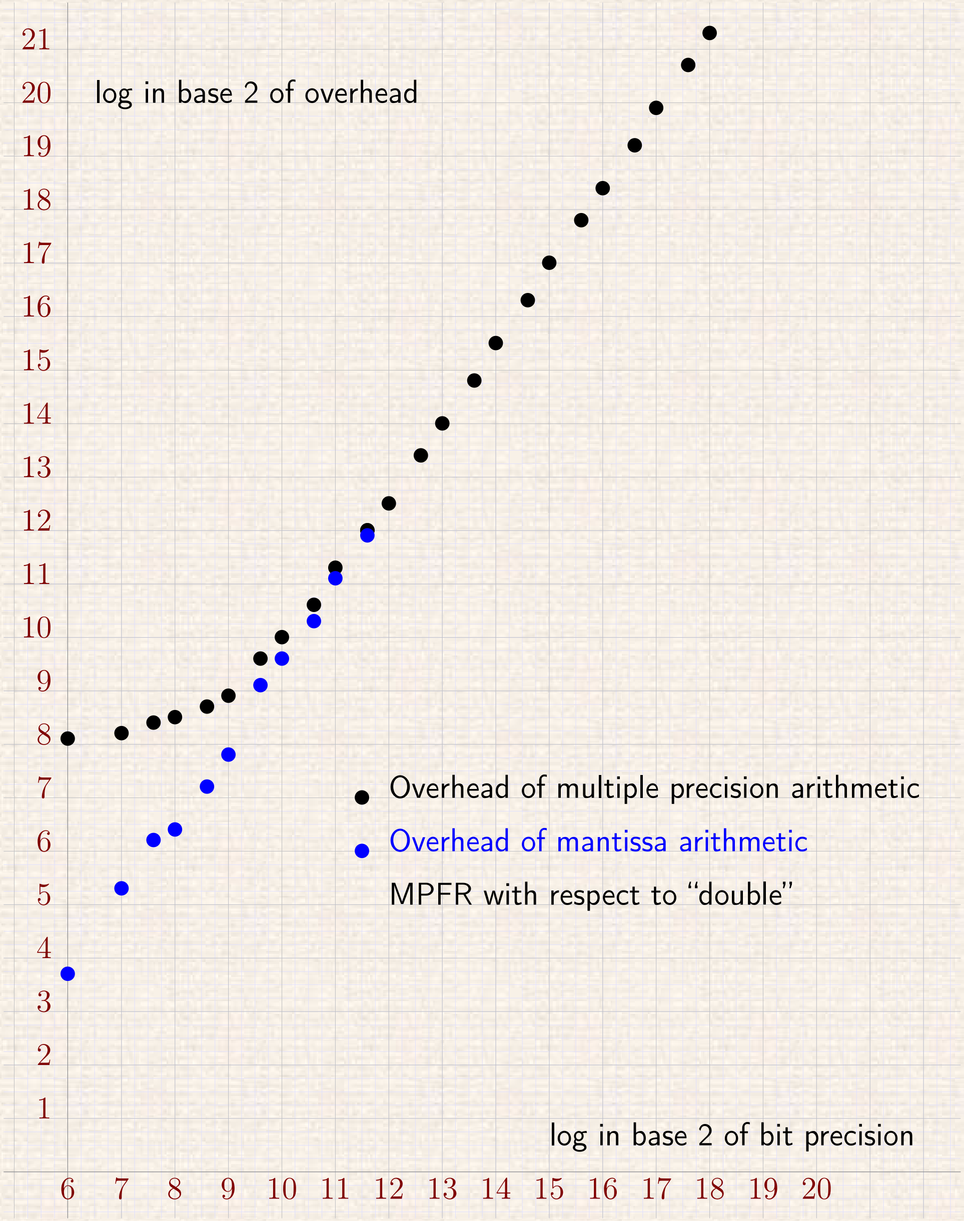
Analysis: computation of $\alpha, a_0, b_0, \ldots, a_{k-1}, b_{k-1}$ yields α with relative error $\approx N^{-k}$
However: we need a precision p with $2^{-p} \lessapprox N^{-2k}$, i.e. $p \geqslant 2\, p_\varepsilon + o(p_\varepsilon)$
Choice of N: depends and to be analyzed in detail

Mathematical simulations

Remark. Multiple precision computations can be particularly useful in order to “simulate” an equation with simple exact mathematical boundary conditions.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Overhead of multiple precision arithmetic
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MPFR with respect to "double"
log in base 2 of bit precision
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What the hardware provides

195*, 196*, 197*: software implementation of floating point arithmetic

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Software implementation, strategy I

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Problem: hardware implementation of three sum

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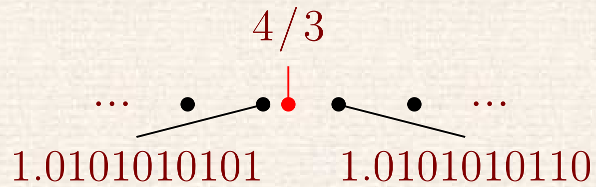
Using built-in floating point arithmetic

Correct rounding



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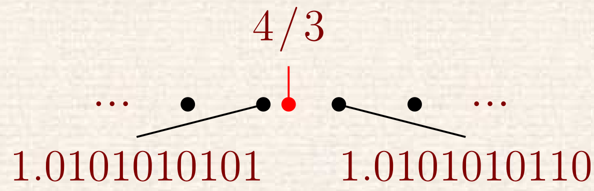

Fused multiply subtract

Problem: exact multiplication of $x, y \in \mathbb{F}_{52}$ as $x\,y = h + l \in \mathbb{F}_{104}$ with $h, l \in \mathbb{F}_{52}$

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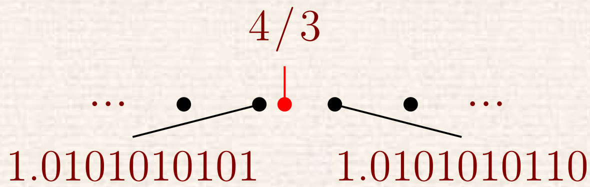

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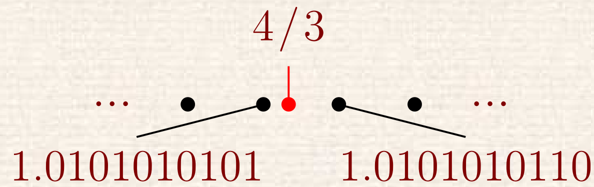

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Three sum (fused add subtract)

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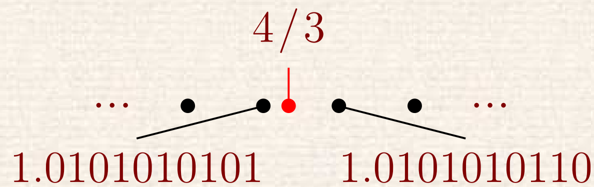

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Exercise

Design multiple precision arithmetic using these operations

Using built-in integer arithmetic

MPFR library

Represent mantissas by GMP integers (with separate field for signs)

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Unsigned fixed point arithmetic

$X \in \{0, \ldots, 2^p - 1\}$ represents $x = X\, 2^{-p}$

Multiplication at precision $2\,p$:

$$(X_1\, 2^p + X_0)\,(Y_1\, 2^p + Y_0)\, 2^{-4p} = X_0\, X_1\, 2^{-2p} + (X_0\, Y_1 + X_1\, Y_0)\, 2^{-3p} + \cdots$$

That is: three integer multiplications and four additions

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Signed fixed point arithmetic

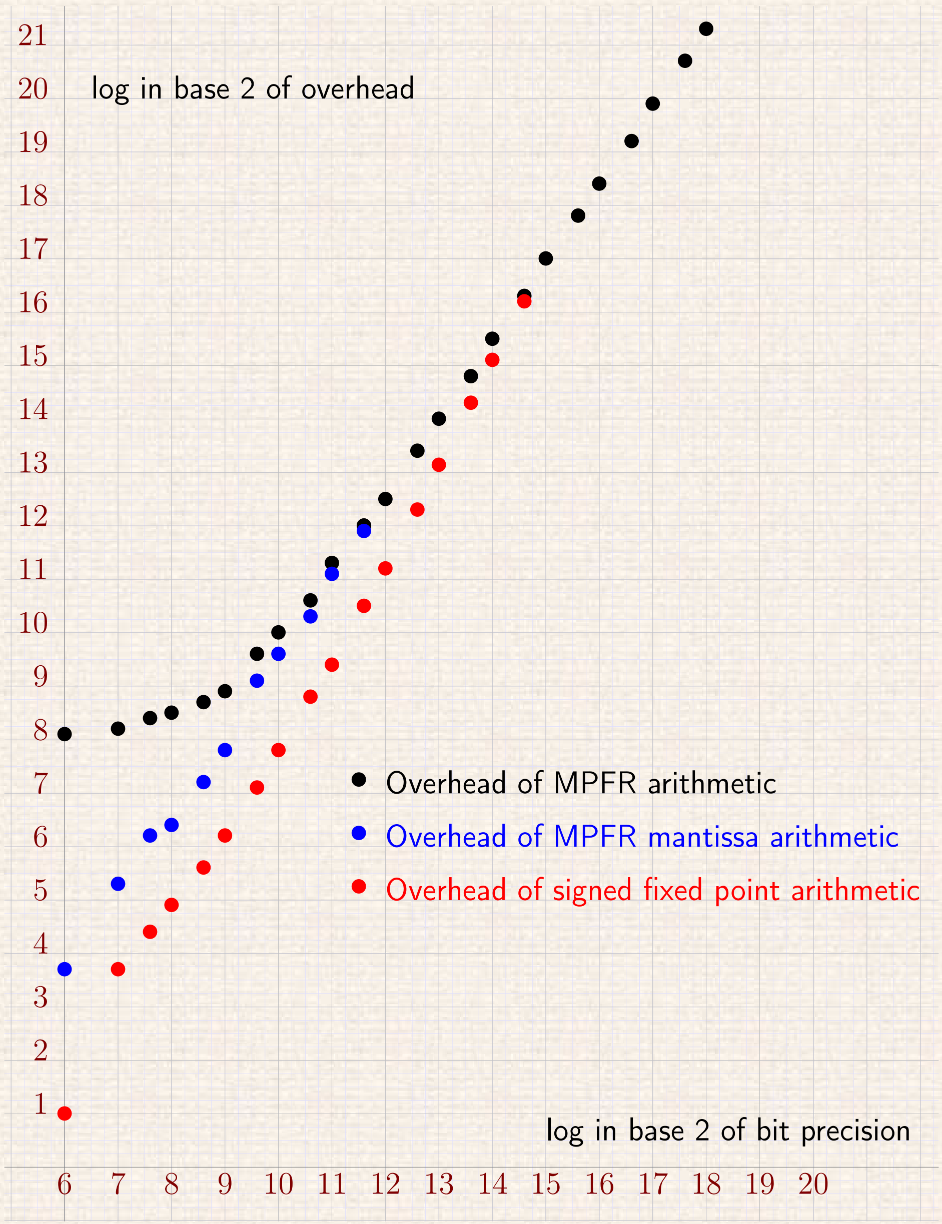
$X \in \{0, \ldots, 2^p - 1\}$ represents $\tilde{x} = X\,2^{-p} - \frac{1}{2}$

$$2\,\tilde{x}\,\tilde{y} + \frac{1}{2} \;=\; 2\,x\,y - (x + y) + 1$$

Multiplication at precision $2\,p$: six extra additions

Moderate precision arithmetic

Precision	Unsigned	Signed	Multipl.
p	1	2	1
$2\,p$	7	13	3
$3\,p$	12	21	6
$4\,p$	18	30	10
$5\,p$	25	40	15
$6\,p$	33	51	21
$7\,p$	42	63	28
$8\,p$	52	76	36



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Rethinking scientific computation

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Challenge 6: how to interface with symbolic computation?

Claim: we can do all our computations using the signed fixed point representation

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Indeed:

- Assume that we want to transform $a_0, \ldots, a_{n-1}$ with $n = 2^k$
- Write $b_i = \frac{a_i}{2\,n\,\|a\|}$ with $\|a\| = \max_i |a_i|$, so that $\hat{a}_i = 2\,n\,\|a\|\,\hat{b}_i$
- Then all numbers occurring in the FFT are in $\left[-\frac{1}{2}, \frac{1}{2}\right]$

Dynamical systems near singularities

The system to integrate

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Preconditioning for signed fixed point arithmetic

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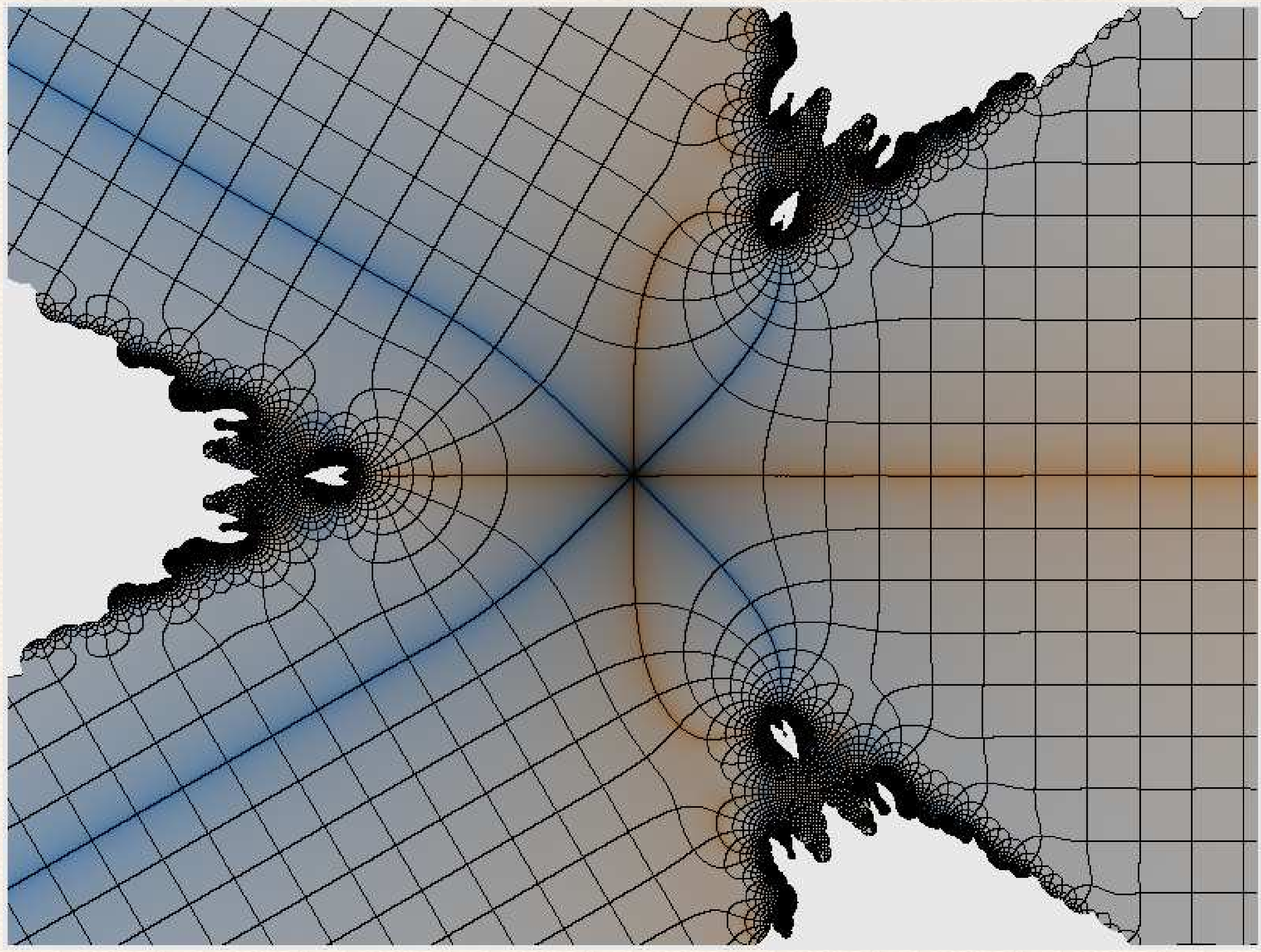
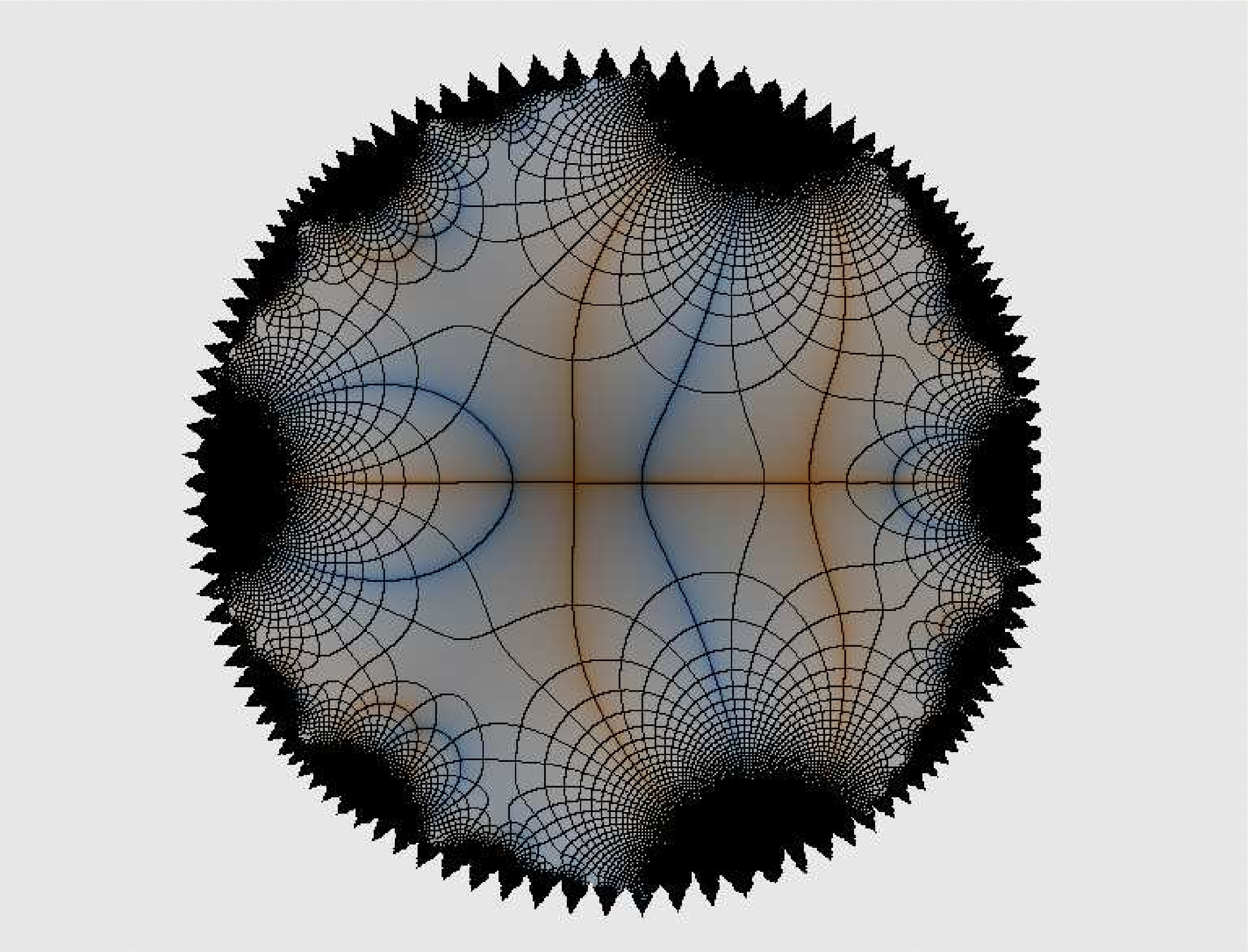
\begin{aligned}
Y(z) &= \tilde{Y}(\varrho z) \\
\tilde{Y}' &= \varrho \Phi(\tilde{Y})
\end{aligned}
$$

Blasius equation



Chazy equation



Matrix multiplication over $\mathbb{Z}$

Problem

Given $M, N \in \mathbb{Z}_{;p}^{n \times n}$, $\mathbb{Z}_{;p} = \{-2^{p-1}, ..., 0, ..., 2^{p-1} - 1\}$, compute MN

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Chinese remaindering when $p \ll n$

- Pick primes $q_1, \ldots, q_l$ with $q_1 \cdots q_l > n\, 2^p$
- Reduce M and N modulo q_i for each i ($O(n^2\, p \log p \log \log p)$ operations)
- Multiply $(M N \bmod q_i) = (M \bmod q_i)\,(N \bmod q_i)$ for each i ($O(n^3\, p)$ operations)
- Reconstruct $M N$ from the $M N \bmod q_i$ ($O(n^2\, p \log^2 p \log \log p)$ operations)

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FFT over a finite field $\mathbb{F}_q$ when $p \not\ll n$

- Pick $q = 3 \times 2^{30} + 1$ and $\omega = 125$ with $\omega^{2^{29}} = -1$ in $\mathbb{F}_q$
- Write integers in base 2^k with $n\, 2^{2k} < q$, i.e. as evaluations $P(2^k)$, $P \in \mathbb{Z}_{;k}[2^k]$
- Compute products of polynomials $P, Q \in \mathbb{Z}_{;k}[2^k]^{n \times n}$ using FFT w.r.t. ω over $\mathbb{F}_q$
- Cost: $O(n^2\, p \log p \log \log p + n^3\, p)$

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Also: no need for a complete theory or big computers
one can start building useful basic libraries for FFT, linear algebra, ...