GPU Accelerated Newton's Method for Taylor Series

1. Overview
   - evaluation and differentiation
   - linearization of power series
2. Data Staging for Evaluation and Differentiation
   - accelerated convolutions
   - data staging algorithms
   - computational results
3. Accelerated Newton's Method
   - solving a triangular block Toeplitz system
   - setup and scalability parameters
   - staggered computations

MCS 572 Lecture 38
Introduction to Supercomputing
Jan Verschelde, 22 November 2024

GPU Accelerated Newton Method for Taylor Series

1. Overview
   - evaluation and differentiation
   - linearization of power series
2. Data Staging for Evaluation and Differentiation
   - accelerated convolutions
   - data staging algorithms
   - computational results
3. Accelerated Newton's Method
   - solving a triangular block Toeplitz system
   - setup and scalability parameters
   - staggered computations

problem statement and overview

Given is

1. a system of polynomials in several variables, where the coefficients are truncated power series in one variable; and
2. one vector of truncated power series as an approximate solution.

Assumption: the problem is regular, the series are Taylor series.

The difficulty of running Newton's method is determined by

1. N, the number of polynomials in the system;
2. n, the number of variables in each polynomial;
3. d, the degree of truncation of the series; and
4. ϵ, the working precision.

Acceleration on a Graphics Processing Unit

The main questions concerning the scalability are below.

1. What are the dimensions (N, n, d, ϵ) to fully occupy the GPU?
2. What is the cost of evaluation and differentiation on a GPU compared to the overall cost of one Newton step?
3. Can GPU acceleration compensate for the cost overhead caused by multiple double arithmetic? For which ϵ?

GPU Accelerated Newton Method for Taylor Series

1. Overview
   - evaluation and differentiation
   - linearization of power series
2. Data Staging for Evaluation and Differentiation
   - accelerated convolutions
   - data staging algorithms
   - computational results
3. Accelerated Newton's Method
   - solving a triangular block Toeplitz system
   - setup and scalability parameters
   - staggered computations

linearization of power series

Working with truncated power series, computing modulo $O(t^d)$, is doing arithmetic over the field of formal series $\mathbb{C}[[t]]$.

Linearization: consider $\mathbb{C}^n[[t]]$ instead of $\mathbb{C}[[t]]^n$. Instead of a vector of power series, we consider a power series with vectors as coefficients.

Solve $\mathbf{A}\mathbf{x} = \mathbf{b}$, $\mathbf{A} \in \mathbb{C}^{n \times n}[[t]]$, $\mathbf{b}, \mathbf{x} \in \mathbb{C}^n[[t]]$. For example:

$$\begin{bmatrix} A_0 & & & \\ A_1 & A_0 & & \\ A_2 & A_1 & A_0 & \\ A_3 & A_2 & A_1 & A_0 \end{bmatrix} \begin{bmatrix} \mathbf{x}_0 \\ \mathbf{x}_1 \\ \mathbf{x}_2 \\ \mathbf{x}_3 \end{bmatrix} = \begin{bmatrix} \mathbf{b}_0 \\ \mathbf{b}_1 \\ \mathbf{b}_2 \\ \mathbf{b}_3 \end{bmatrix}$$

linearizes $\mathbf{A}(t)\mathbf{x}(t) = \mathbf{b}(t)$, with

$$\begin{aligned} \mathbf{A}(t) &= A_0 + A_1 t + A_2 t^2 + A_3 t^3, \\ \mathbf{x}(t) &= \mathbf{x}_0 + \mathbf{x}_1 t + \mathbf{x}_2 t^2 + \mathbf{x}_3 t^3, \quad \mathbf{b}(t) = \mathbf{b}_0 + \mathbf{b}_1 t + \mathbf{b}_2 t^2 + \mathbf{b}_3 t^3. \end{aligned}$$

GPU Accelerated Newton Method for Taylor Series

1. Overview
   - evaluation and differentiation
   - linearization of power series
2. Data Staging for Evaluation and Differentiation
   - accelerated convolutions
   - data staging algorithms
   - computational results
3. Accelerated Newton's Method
   - solving a triangular block Toeplitz system
   - setup and scalability parameters
   - staggered computations

accelerated convolutions

$\left(x_0 + x_1 t + \cdots + x_d t^d\right) \star \left(y_0 + y_1 t + \cdots + y_d t^d\right)$ has coefficients

$$z_k = \sum_{i=0}^{k} x_i \cdot y_{k-i}, \quad k = 0, 1, \ldots, d.$$

Thread k computes z_k.

To avoid thread divergence, pad with zeros, e.g. for $d = 3$:

X	x_0	x_1	x_2	x_3				
Y	0	0	0	0	y_0	y_1	y_2	y_3
Z	z_0	z_1	z_2	z_3				

The arrays X, Y, and Z are in shared memory.

pseudo code for a convolution kernel

Thread k computes $z_k = \sum_{i=0}^{k} x_i \cdot y_{k-i}, k = 0, 1, \ldots, d,$

after loading the coefficients into shared memory arrays

X	x_0	x_1	x_2	x_3				
Y	0	0	0	0	y_0	y_1	y_2	y_3
Z	z_0	z_1	z_2	z_3				

1. $X_k := x_k$
2. $Y_k := 0$
3. $Y_{d+k} := y_k$
4. $Z_k := X_0 \cdot Y_{d+k}$
5. for i from 1 to d do $Z_k := Z_k + X_i \cdot Y_{d+k-i}$
6. $z_k := Z_k$

evaluating and differentiating one monomial

Evaluating and differentiating $a x_1 x_2 x_3 x_4 x_5$ at a power series vector:

$$
\begin{array}{lll}
f_1 := a \star z_1 & b_1 := z_5 \star z_4 & \\
f_2 := f_1 \star z_2 & b_2 := b_1 \star z_3 & \\
f_3 := f_2 \star z_3 & b_3 := b_2 \star z_2 & c_1 := f_1 \star b_2 \\
f_4 := f_3 \star z_4 & b_3 := b_3 \star a & c_2 := f_2 \star b_1 \\
f_5 := f_4 \star z_5 & & c_3 := f_3 \star z_5
\end{array}
$$

- The gradient is in $(b_3, c_1, c_2, c_3, f_4)$ and the value is in f_5.
- Each $\star$ is a convolution between two truncated power series.
- Statements on the same line can be computed in parallel.

Given sufficiently many blocks of threads,
monomial evaluation and differentiation takes n steps for n variables.

accelerated algorithmic differentiation

$$
\begin{array}{rcccccc}
p & = & a_0 + & a_1 x_1 x_3 x_6 & + & a_2 x_1 x_2 x_5 x_6 & + & a_3 x_2 x_3 x_4 \\
 & & & f_{1,1} := a_1 \star z_1 & & f_{2,1} := a_2 \star z_1 & & f_{3,1} := a_3 \star z_2 \\
 & & & f_{1,2} := f_{1,1} \star z_3 & & f_{2,2} := f_{2,1} \star z_2 & & f_{3,2} := f_{3,1} \star z_3 \\
 & & & f_{1,3} := f_{1,2} \star z_6 & & f_{2,3} := f_{2,2} \star z_5 & & f_{3,3} := f_{3,2} \star z_4 \\
 & & & & & f_{2,4} := f_{2,3} \star z_6 & & \\
 & & & b_{1,1} := z_6 \star z_3 & & b_{2,1} := z_6 \star z_5 & & b_{3,1} := z_4 \star z_3 \\
 & & & b_{1,1} := b_{1,1} \star a_1 & & b_{2,2} := b_{2,1} \star z_2 & & b_{3,1} := b_{3,1} \star a_3 \\
 & & & & & b_{2,2} := b_{2,2} \star a_2 & & \\
 & & & c_{1,1} := f_{1,1} \star z_6 & & c_{2,1} := f_{2,1} \star b_{2,1} & & c_{3,1} := f_{3,1} \star z_4 \\
 & & & & & c_{2,2} := f_{2,2} \star z_6 & &
\end{array}
$$

The 21 convolutions are arranged below (on same line: parallel execution):

$$
\begin{array}{cccccccccc}
f_{1,1} & b_{1,1} & & f_{2,1} & b_{2,1} & & f_{3,1} & b_{3,1} & & \\
f_{1,2} & b_{1,1} & c_{1,1} & f_{2,2} & b_{2,2} & c_{2,1} & f_{3,2} & b_{3,1} & c_{3,1} & \\
f_{1,3} & & & f_{2,3} & b_{2,2} & c_{2,2} & f_{3,3} & & & \\
 & & & f_{2,4} & & & & & &
\end{array}
$$

GPU Accelerated Newton Method for Taylor Series

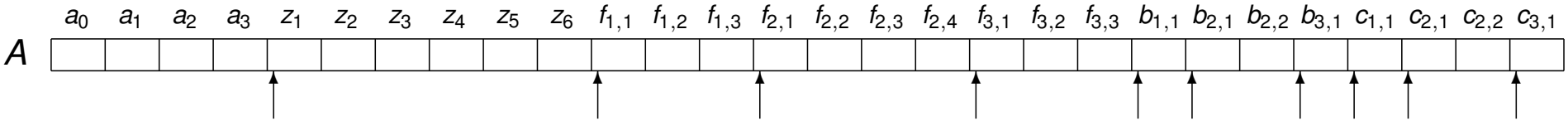
1. Overview
   - evaluation and differentiation
   - linearization of power series
2. Data Staging for Evaluation and Differentiation
   - accelerated convolutions
   - data staging algorithms
   - computational results
3. Accelerated Newton's Method
   - solving a triangular block Toeplitz system
   - setup and scalability parameters
   - staggered computations

staging of the data

The 21 convolutions

$$
\begin{array}{cccccccccc}
f_{1,1} & b_{1,1} & & f_{2,1} & b_{2,1} & & f_{3,1} & b_{3,1} & & \\
f_{1,2} & b_{1,1} & c_{1,1} & f_{2,2} & b_{2,2} & c_{2,1} & f_{3,2} & b_{3,1} & c_{3,1} & \\
f_{1,3} & & & f_{2,3} & b_{2,2} & c_{2,2} & f_{3,3} & & & \\
 & & & f_{2,4} & & & & & &
\end{array}
$$

are stored after the power series coefficients a_0, a_1, a_2, a_3,
and the input power series z_1, z_2, z_3, z_4, z_5, z_6 in the array A below:



- The arrows point at the start position of the input series and at the forward $f_{i,j}$, backward $b_{i,j}$, cross products $c_{i,j}$ for every monomial i.
- For complex and multiple double numbers, there are multiple data arrays, for real, imaginary parts, and for each double in a multiple double.

convolution jobs

One block of threads does one convolution.
It takes four kernel launches, to compute the 21 convolutions

$$
\begin{array}{lll}
f_{1,1} & b_{1,1} & \\
f_{1,2} & b_{1,1} & c_{1,1} \\
f_{1,3} & &
\end{array}
\qquad
\begin{array}{lll}
f_{2,1} & b_{2,1} & \\
f_{2,2} & b_{2,2} & c_{2,1} \\
f_{2,3} & b_{2,2} & c_{2,2} \\
f_{2,4} & &
\end{array}
\qquad
\begin{array}{lll}
f_{3,1} & b_{3,1} & \\
f_{3,2} & b_{3,1} & c_{3,1} \\
f_{3,3} & &
\end{array}
$$

respectively with 6, 9, 5, and 1 block of threads.

Given sufficiently many blocks of threads, all convolutions for the polynomial evaluation and differentiation take m steps, where m is the largest number of variables in one monomial.

A convolution job j is defined by the triplet $(t_1(j), t_2(j), t_3(j))$, where

- $t_1(j)$ and $t_2(j)$ are the locations in the array A for the input, and
- $t_3(j)$ is the location in A of the output of the convolution.

addition jobs

One block of threads does one addition of two power series.

An addition job j is defined by the pair $(t_1(j), t_2(j))$, where

- $t_1(j)$ is the location in the array A of the input, and
- $t_2(j)$ is the location in the array A of the update.

Jobs are defined recursively, following the tree summation algorithm.

The job index j corresponds to the block index in the kernel launch.

Given sufficiently many blocks of threads,
polynomial evaluation and differentiation takes $m + \lceil \log_2(N) \rceil$ *steps,*
where m *is the largest number of variables in one monomial*
and N *is the number of monomials.*

For $N \gg m$, an upper bound for the speedup is $dN/\log_2(N)$,
where d is the degree at which the series are truncated.

GPU Accelerated Newton Method for Taylor Series

1. Overview
   - evaluation and differentiation
   - linearization of power series
2. Data Staging for Evaluation and Differentiation
   - accelerated convolutions
   - data staging algorithms
   - computational results
3. Accelerated Newton's Method
   - solving a triangular block Toeplitz system
   - setup and scalability parameters
   - staggered computations

algorithmic differentiation on five different GPUs

Run code generated by the CAMPARY software,
by M. Joldes, J.-M. Muller, V. Popescu, W. Tucker, in ICMS 2016.

on five different GPUs:

NVIDIA GPU	CUDA	#MP	#cores/MP	#cores	GHz
Tesla C2050	2.0	14	32	448	1.15
Kepler K20C	3.5	13	192	2496	0.71
Pascal P100	6.0	56	64	3584	1.33
Volta V100	7.0	80	64	5120	1.91
GeForce RTX 2080	7.5	46	64	2944	1.10

The double peak performance of the P100 is 4.7 TFLOPS.
At 7.9 TFLOPS, the V100 is 1.68 times faster than the P100.

To evaluate the algorithms, compare the ratios of the wall clock times on the P100 over V100 with the factor 1.68.

three test polynomials

For each polynomial, p_1, p_2, p_3,

- n is the total number of variables,
- m is the number of variables per monomial, and
- N is the number of monomials (not counting the constant term).

The last two columns list the number of convolution and addition jobs:

	n	m	N	#cnv	#add
p_1	16	4	1,820	16,380	9,084
p_2	128	64	128	24,192	8,192
p_3	128	2	8,128	24,256	24,256

Does the shape of the test polynomials influence the execution times?

performance of the five GPUs

In evaluating p_1 for degree $d = 152$ in deca double precision, the `cudaEventElapsedTime` measures the times of kernel launches. The last line is the wall clock time for all convolution and addition kernels. All units are milliseconds.

	C2050	K20C	P100	V100	RTX 2080
convolution	12947.26	11290.22	1060.03	634.29	10002.32
addition	10.72	11.13	1.37	0.77	5.01
sum	12957.98	11301.35	1061.40	635.05	10007.34
wall clock	12964.00	11309.00	1066.00	640.00	10024.00

- The $12964/640 \approx 20.26$ is for the V100 over the oldest C2050.
- Compare the ratio of the wall clock times for P100 over V100 $1066/640 \approx 1.67$ with the ratios of theoretical double peak performance of the V100 of the P100: $7.9/4.7 \approx 1.68$.

teraflop performance

In 1.066 second, the P100 did 16,380 convolutions, 9,084 additions.

- One convolution on series truncated at degree d requires $(d+1)^2$ multiplications and $d(d+1)$ additions.
- One addition of two series at degree d requires $d+1$ additions.

So we have $16,380(d+1)^2$ multiplications and
$16,380d(d+1) + 9,084(d+1)$ additions in deca double precision.

- One multiplication and one addition in deca double precision require respectively 3,089 and 397 double operations.
- The $16,380(d+1)^2$ evaluates to 1,184,444,368,380 and $16,380d(d+1) + 9,084(d+1)$ to 151,782,283,404 operations.

In total, in 1.066 second the P100 did 1,336,226,651,784 double float operations, reaching a performance of 1.25 TFLOPS.

scalability

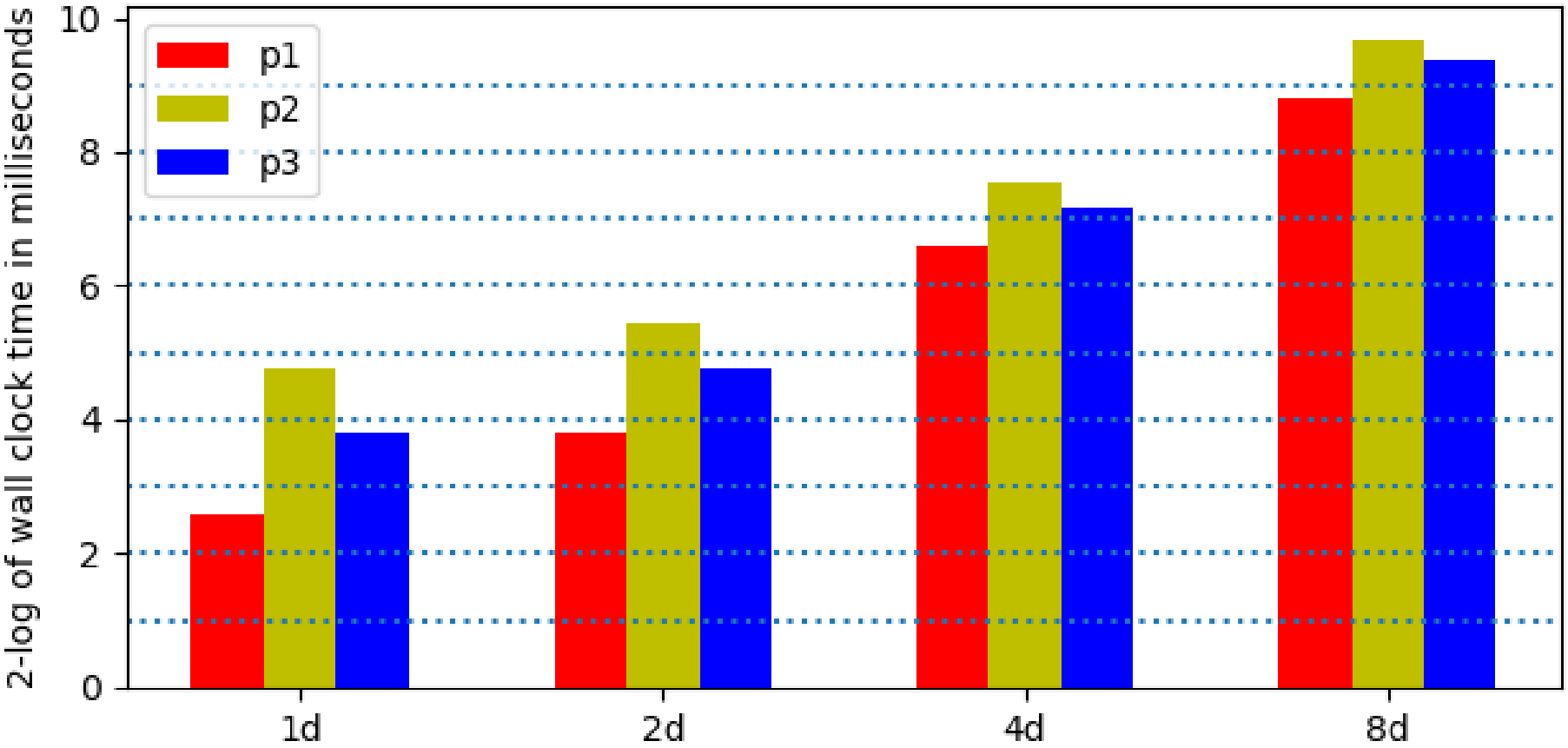
To examine the scalability, consider

1. the doubling of the precision, in double, double double, quad double and octo double precision, for fixed degree 191; and
2. the doubling of the number of coefficients of the series, from 32 to 64, and from 64 to 128.

For increasing precision, the problem becomes more compute bound.

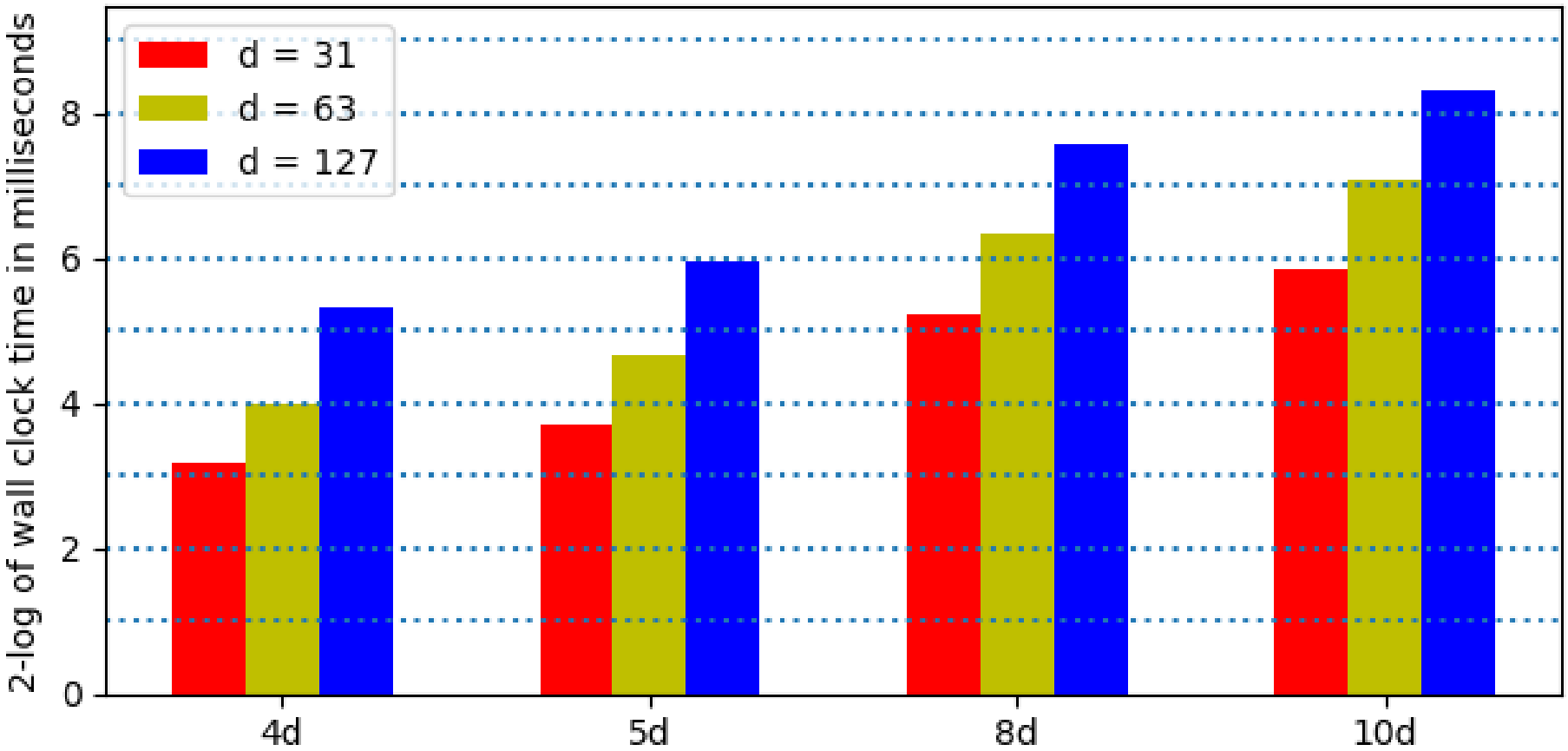
doubling the precision

The 2-logarithm of the wall clock times to evaluate and differentiate p_1, p_2, p_3 in double (1d), double double (2d), quad double (4d), and octo double (8d) precision, for power series truncated at degree 191:



doubling the number of coefficients of the series

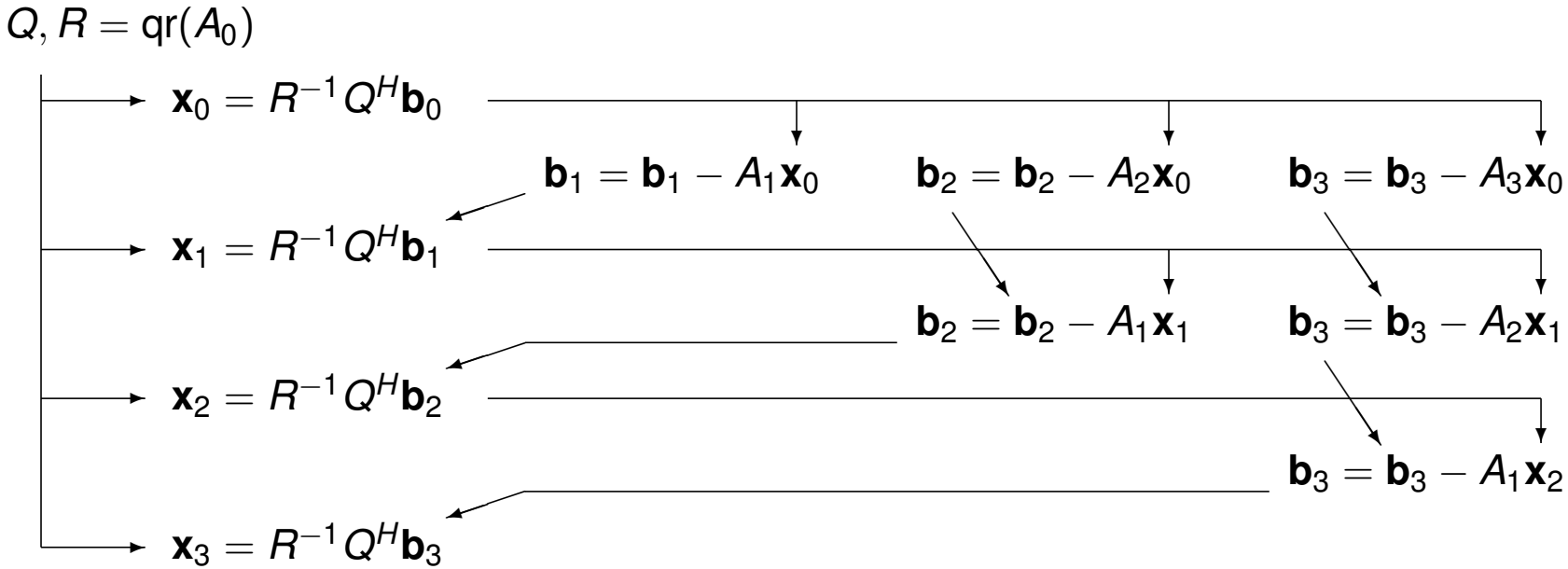
The 2-logarithm of the wall clock times to evaluate and differentiate p_1 in quad double (4d), penta double (5d), octo double (8d), and deca double (10d) precision, for power series of degrees 31, 63, and 127:



GPU Accelerated Newton Method for Taylor Series

1. Overview
   - evaluation and differentiation
   - linearization of power series
2. Data Staging for Evaluation and Differentiation
   - accelerated convolutions
   - data staging algorithms
   - computational results
3. Accelerated Newton's Method
   - solving a triangular block Toeplitz system
   - setup and scalability parameters
   - staggered computations

a task graph for a triangular block Toeplitz system



$$\begin{bmatrix} A_0 & & & \\ A_1 & A_0 & & \\ A_2 & A_1 & A_0 & \\ A_3 & A_2 & A_1 & A_0 \end{bmatrix} \begin{bmatrix} \mathbf{x}_0 \\ \mathbf{x}_1 \\ \mathbf{x}_2 \\ \mathbf{x}_3 \end{bmatrix} = \begin{bmatrix} \mathbf{b}_0 \\ \mathbf{b}_1 \\ \mathbf{b}_2 \\ \mathbf{b}_3 \end{bmatrix}$$

linearizes $A(t)\mathbf{x}(t) = \mathbf{b}(t)$, with

$$\begin{aligned} A(t) &= A_0 + A_1 t + A_2 t^2 + A_3 t^3, \\ \mathbf{x}(t) &= \mathbf{x}_0 + \mathbf{x}_1 t + \mathbf{x}_2 t^2 + \mathbf{x}_3 t^3, \quad \mathbf{b}(t) = \mathbf{b}_0 + \mathbf{b}_1 t + \mathbf{b}_2 t^2 + \mathbf{b}_3 t^3. \end{aligned}$$

GPU Accelerated Newton Method for Taylor Series

1. Overview
   - evaluation and differentiation
   - linearization of power series
2. Data Staging for Evaluation and Differentiation
   - accelerated convolutions
   - data staging algorithms
   - computational results
3. Accelerated Newton's Method
   - solving a triangular block Toeplitz system
   - setup and scalability parameters
   - staggered computations

monomial homotopies

Consider n variables $\mathbf{x}$, A is an n-by-n exponent matrix, and $\mathbf{b}(t)$ is a vector of n series of order $O(t^d)$:

$$\mathbf{x}^A = \mathbf{b}(t) \quad \text{is a } \textit{monomial homotopy}.$$

For example, $n = 3$, $\mathbf{x} = [x_1, x_2, x_3]$:

$$A = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 1 \end{bmatrix} \quad \begin{cases} x_1 = b_1(t) & x_1(t) = \exp(\alpha_1 t) + O(t^d) \\ x_1 x_2 = b_2(t) & x_2(t) = \exp(\alpha_2 t) + O(t^d) \\ x_1 x_2 x_3 = b_3(t) & x_3(t) = \exp(\alpha_3 t) + O(t^d) \end{cases}$$

where

$$\exp(\alpha t) + O(t^4) = 1 + \alpha t + \frac{\alpha^2}{2!} t^2 + \frac{\alpha^3}{3!} t^3 + O(t^4),$$

with $\alpha \in [-1, -1+\delta] \cup [1-\delta, 1]$, $\delta > 0$, or $|\alpha| = 1$ for random $\alpha \in \mathbb{C}$.

order of series, accuracy and precision

$$\exp(t) = \sum_{k=0}^{d-1} \frac{t^k}{k!} + O(t^d)$$

k	$1/k!$	recommended precision
7	2.0e-004	double precision okay
15	7.7e-013	use double doubles
23	3.9e-023	use double doubles
31	1.2e-034	use quad doubles
47	3.9e-060	use octo doubles
63	5.0e-088	use octo doubles
95	9.7e-149	need hexa doubles
127	3.3e-214	need hexa doubles

scalability parameters

1. Going from one to two columns of monomials:

$$\mathbf{c}_1 \mathbf{x}^{A_1} + \mathbf{c}_2 \mathbf{x}^{A_2} = \mathbf{b}(t),$$

   for two n-vectors $\mathbf{c}_1$ and $\mathbf{c}_2$ and two exponent matrices A_1 and A_2.
2. For increasing dimensions: $n = 64, 128, 256, 512, 1024$.
3. For increasing orders d in $O(t^d)$, $d = 1, 2, 4, 8, 16, 32, 64$.
4. For increasing precision:
   double, double double, quad double, octo double.

Doubling columns, dimensions, orders, and precision,
how much of the overhead can be compensated by GPU acceleration?

GPU Accelerated Newton Method for Taylor Series

1. Overview
   - evaluation and differentiation
   - linearization of power series
2. Data Staging for Evaluation and Differentiation
   - accelerated convolutions
   - data staging algorithms
   - computational results
3. Accelerated Newton's Method
   - solving a triangular block Toeplitz system
   - setup and scalability parameters
   - staggered computations

different types of accelerated computations

1. convolutions for evaluation and differentiation
2. Householder QR
3. $Q^H\mathbf{b}$ computations
4. back substitutions to solve $R\mathbf{x} = Q^H\mathbf{b}$
5. updates $\mathbf{b} = \mathbf{b} - A\mathbf{x}$
6. residual computations $\|\mathbf{b} - A\mathbf{x}\|_1$

Which of the six types occupies most time?

staggered computations

Computing $\mathbf{x}(t) = \mathbf{x}_0 + \mathbf{x}_1 t + \mathbf{x}_2 t^2 + \cdots + \mathbf{x}_{d-1} t^{d-1}$, observe:

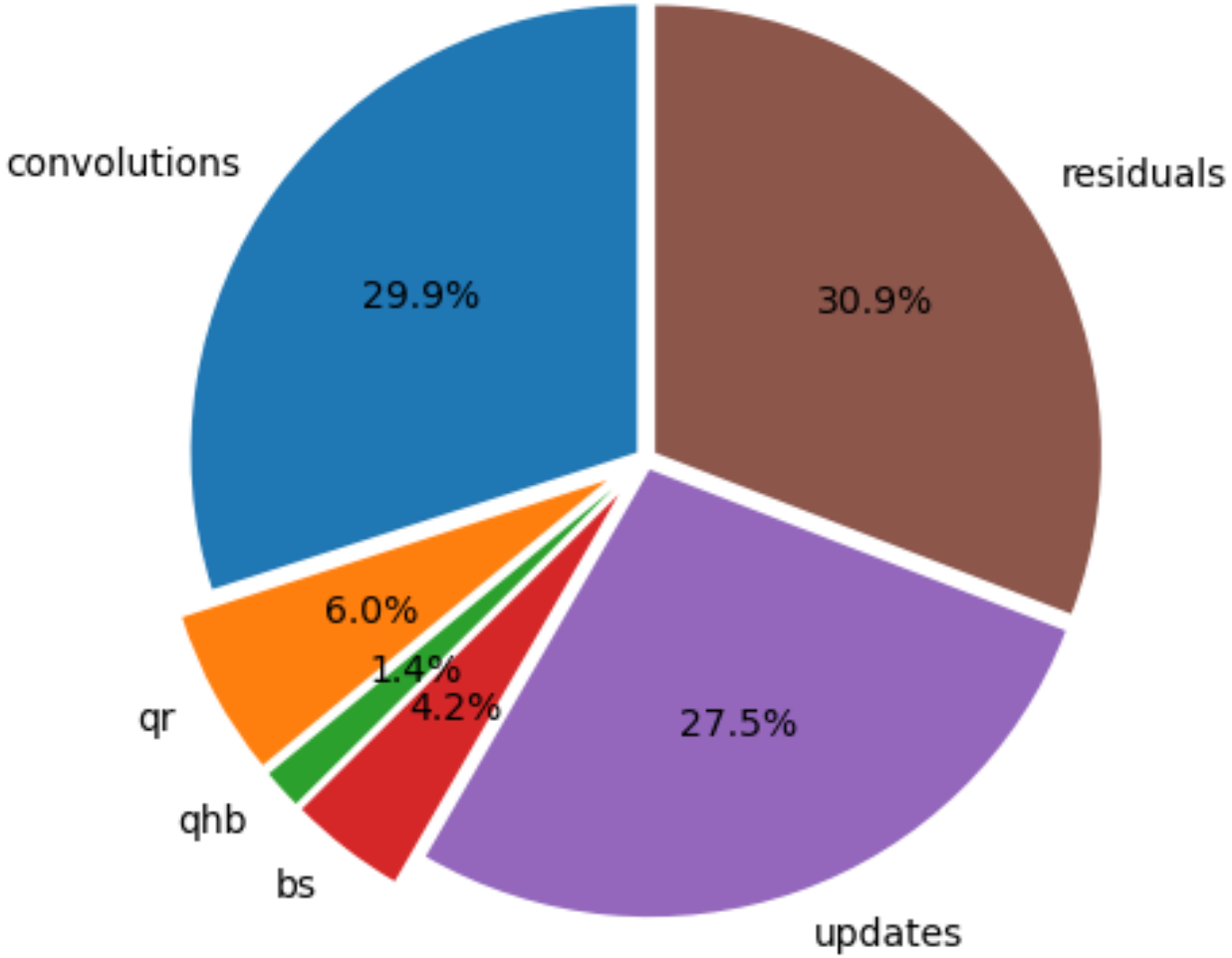
1. Start $\mathbf{x}_0$ with half its precision correct,
   otherwise Newton's method may not converge.
2. Increase d in the order $O(t^d)$ gradually,
   e.g.: the new d is $d + 1 + d/2$,
   hoping (at best) for quadratic convergence.
3. Once $\mathbf{x}_k$ is correct, the corresponding $\mathbf{b}_k = 0$,
   as $\mathbf{b}_k$ is obtained by evaluation, and then the update $\Delta\mathbf{x}_k$ should no longer be computed because

$$QR\Delta\mathbf{x}_k = \mathbf{b}_k = \mathbf{0} \quad \Rightarrow \quad \Delta\mathbf{x}_k = \mathbf{0}.$$

   This gives a criterion to stop the iterations.

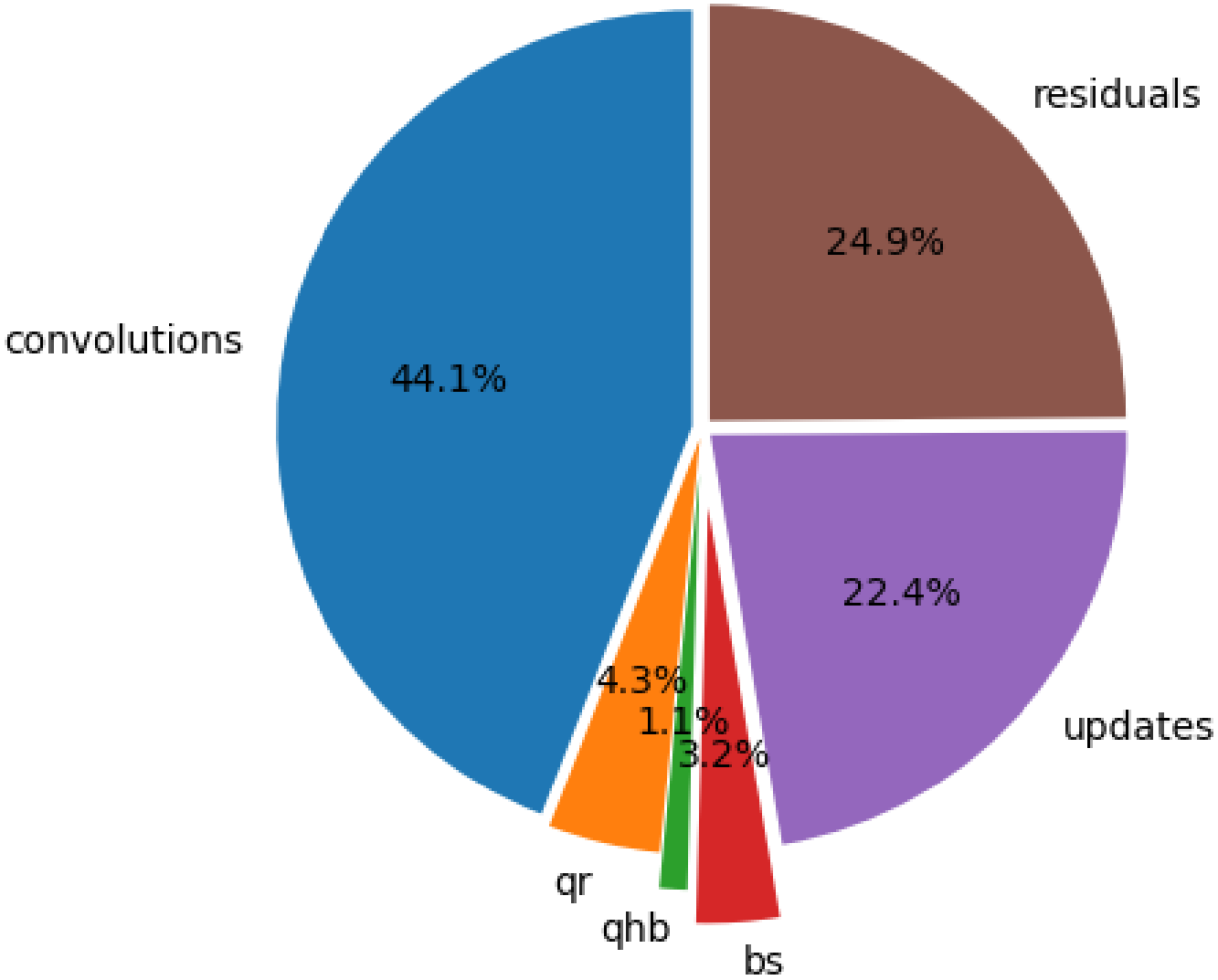
$n = 1024$, $d = 64$, 24 steps in octo double precision

On one column of monomials, triangular exponent matrix of ones.
Six different types of accelerated computations, on the V100.



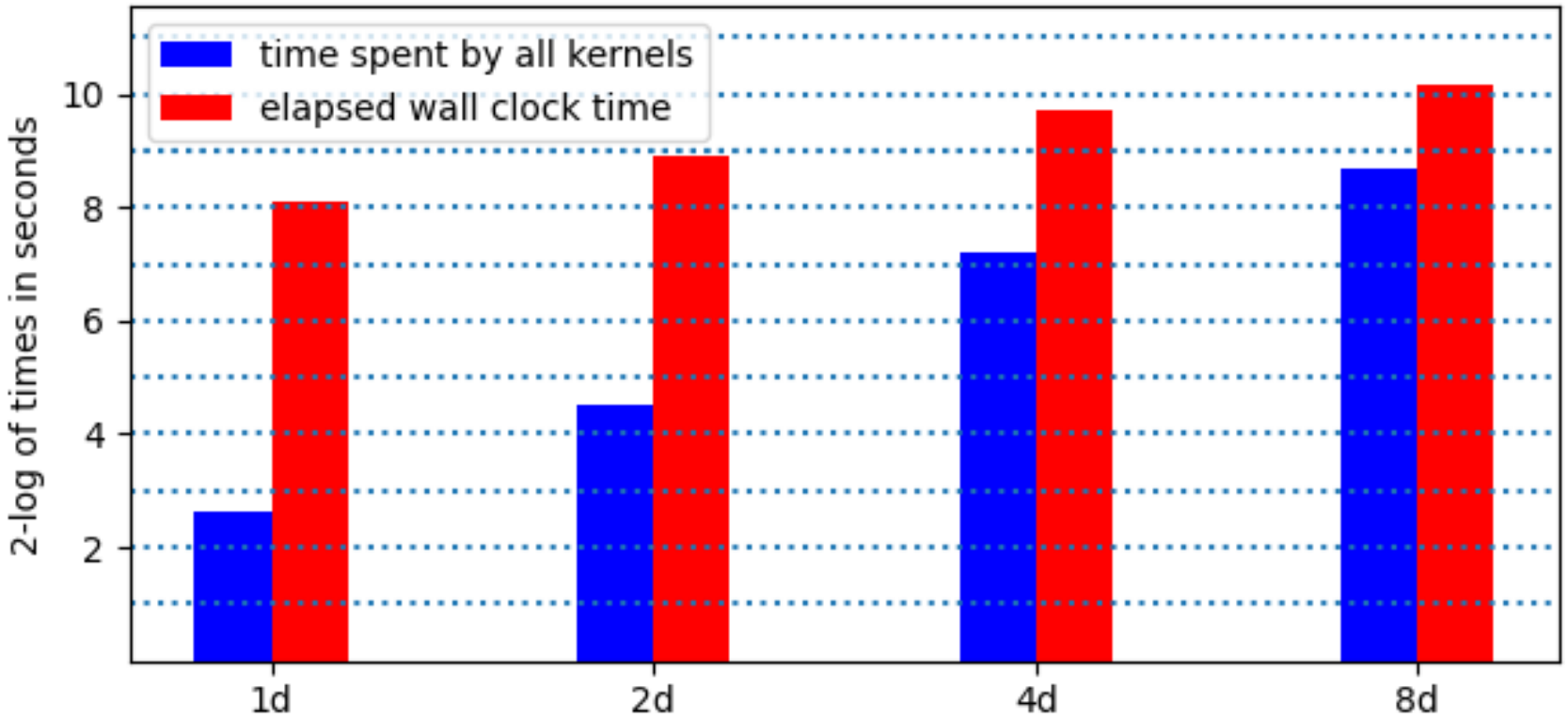
$n = 1024$, $d = 64$, 24 steps in octo double precision

On *two* columns of monomials, triangular exponent matrix of ones.
Six different types of accelerated computations, on the V100.



doubling precisions, wall clock and kernel times

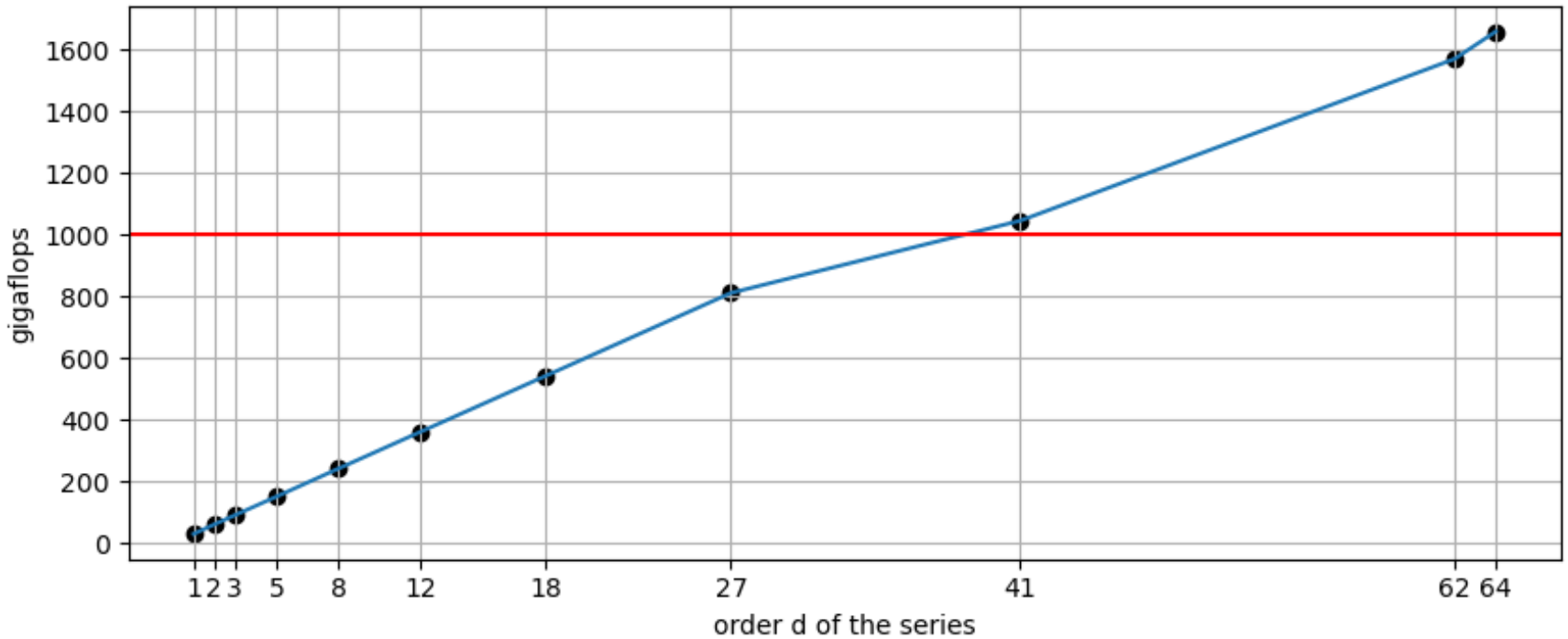
On one column of monomials, triangular exponent matrix of ones, $n = 1024$, $d = 64$, 24 steps, in 4 different precisions, on the V100:



Doubling the precision less than doubles the wall clock time and increases the time spent by all kernels.

teraflop performance of convolutions

On one column of monomials, triangular exponent matrix of ones,
$n = 1024$, performance of the evaluation and differentiation,
in octo double precision, for increasing orders of the series:



After degree 40, teraflop performance is observed on the V100.

three publications and code

- **Accelerated polynomial evaluation and differentiation at power series in multiple double precision.**
  In the *2021 IEEE International Parallel and Distributed Processing Symposium Workshops (IPDPSW)*, pages 740–749. IEEE, 2021. `arXiv:2101.10881`
- **Least squares on GPUs in multiple double precision.**
  In the *2022 IEEE International Parallel and Distributed Processing Symposium Workshops (IPDPSW)*, pages 828–837. IEEE, 2022. `arXiv:2110.08375`
- **GPU Accelerated Newton for Taylor Series Solutions of Polynomial Homotopies in Multiple Double Precision.**
  In the *Proceedings of the 26th International Workshop on Computer Algebra in Scientific Computing (CASC 2024)*, pages 328–348. Springer, 2024. `arXiv:2301.12659`

Code at `github.com/janverschelde/PHCpack`, GPL-3.0 License.