GPU-ACCELERATED PATH TRACKER FOR POLYHEDRAL HOMOTOPY

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Abstract. The polyhedral homotopy method of Huber and Sturmfels is a particularly efficient and robust numerical method for solving system of (Laurent) polynomial equations. A central component in an implementation of this method is an efficient and scalable path tracker. While the implementation issues in a scalable path tracker for computer clusters or multi-core CPUs have been solved thoroughly, designing good GPU-based implementations is still an active research topic. This paper addresses the core issue of efficiently evaluate a multivariate system of Laurent polynomials together with all its partial derivatives. We propose a simple approach that maps particularly well onto the parallel computing architectures of modern GPUs. As a by-product, we also simplify and accelerate the path tracker by consolidating the computation of Euler and Newton directions.

1. Introduction

Numerical homotopy continuation methods have emerged as a robust and efficient family of numerical methods for solving systems of polynomial equations \cite{1,8,18}. Their most salient advantage is that each solution can be computed independently making such methods pleasantly parallel. A great variety of specific homotopy constructions have been proposed. In their seminal work \cite{12}, Huber and Sturmfels introduced the particularly attractive polyhedral homotopy method, which can take full advantage of the Newton polytope structure of the target system. The implementation of polyhedral homotopy on computer clusters and multi-core CPUs has been explored thoroughly. This paper addresses the unique challenges in leveraging the power of GPUs and similar devices.

Central to the polyhedral homotopy method (and homotopy methods in general) are the “path tracking” algorithms for tracking the homotopy paths. While a great variety of numerical methods can be used for path tracking, the predictor-corrector scheme has emerged as the method of choice within the community of numerical homotopy methods due to its superior efficiency and stability \cite{1,16,19}. For a typical predictor-corrector based path tracker, a significant portion of computation time is devoted to the evaluation of the homotopy function together with its partial derivatives. Indeed, this part may dominate the overall computational cost in the path tracking process for systems having complicated expressions relative to its dimension. The simultaneous evaluation of a (multivariate) system of polynomial functions given by the polyhedral homotopy construction together with all its partial derivatives is our main focus. Tremendous efforts have been devoted to this problem within the community of polyhedral homotopy method (e.g. \cite{13,15,20,21}) as well as the community of the homotopy method in general. In the broader context, this is the main subject of the established field of Automatic Differentiation \cite{10}.

In the present contribution we propose a very simple approach for efficiently evaluating a homotopy function together with all its partial derivatives, in the context the polyhedral homotopy method, that is particularly efficient in modern GPUs and similar devices. Indeed, the problem of evaluating Laurent polynomial systems together with their derivatives is converted into general matrix multiplication (GEMM) operations \cite{14}, which modern GPUs (especially the newer designs like the “Tensor Cores” of NVIDIA) are designed to optimize. Grounded on this technique, we also unify the computation of Euler and Newton directions that are needed in path tracking.
2. A REVIEW OF POLYHEDRAL HOMOTOPY

This section briefly review the polyhedral homotopy of Huber and Sturmfels \[12\]. For simplicity, we first restrict our attention to systems having “generic coefficients” in the sense of the Bernstein’s First Theorem \[2\]. A square Laurent polynomial system in the variables \(x = (x_1, \ldots, x_n)\) is a system \(F = (f_1, \ldots, f_n)\) given by \(f_k(x) = \sum_{a \in S_k} c_{k,a} x^a\) for \(k = 1, \ldots, n\), where the nonempty finite set of column vectors \(S_k \subset \mathbb{Z}^n\) describes the exponents appeared in the monomials in \(f_k\), and the “multi-exponent” notation \(x^a = x_1^{a_1} \cdots x_n^{a_n}\) describes a monomial whose exponents are given by the (column) vector \(a\). The goal is to find all isolated zeros of \(F(x)\) in \((\mathbb{C}^*)^n = (\mathbb{C} \setminus \{0\})^n\). Given lifting functions \(\omega_k : S_k \to \mathbb{Q}^+\) for \(k = 1, \ldots, n\), the polyhedral homotopy of Huber and Sturmfels for solving the target system \(F(x) = 0\) is given by the homotopy function \(H = (h_1, \ldots, h_n)\) with
\[
(1) \quad h_k(x,t) = \sum_{a \in S_k} c_{k,a} x^a t^{-\omega_k(a)} \quad \text{for} \ k = 1, \ldots, n.
\]
Clearly, \(H(x,1) \equiv F(x)\) is exactly the target system. Under the genericity assumption, \(H(x,t) = 0\) defines smooth paths in \((\mathbb{C}^*)^n \times (0,1)\), parametrized by \(t\), emanating from isolated \(\mathbb{C}^*\)-zeros of \(F(x) \equiv H(x,1)\) and continue toward \(t = 0\). Once the starting points of these paths at \(t = 0\) are obtained, the \(\mathbb{C}^*\)-zeros of the target system \(F(x)\) can be found by tracking these paths.

Since the starting points are not directly involved in our discussions, we simply assume the set of all solution to \(H(x,t_0) = 0\) in \((\mathbb{C}^*)^n\) for a common \(t\)-value of \(t = t_0 > 0\), is readily available and refer to Refs. \[12\] for detailed discussions on the step of locating the starting points.

2.1. Logarithmic homotopy parameter. One potential source of numerical instability is the scale of \(\|\partial H/\partial t\|\) near \(t = 0\), which may be infinite. The most widely accepted solution is to use the substitution \(t = e^\tau\) and adopt \(\tau\) as the path parameter \[11, 15\]. The original interval \(t \in (0,1)\) is maps to the corresponding interval \(\tau \in (-\infty,0)\), thus “dilutes” the numerical instability. With this, \(1\) can be reformulated as \(H = (h_1, \ldots, h_n) : (\mathbb{C}^*)^n \times (-\infty,0]\) given by
\[
(2) \quad h_k(x,\tau) = \sum_{a \in S_k} c_{k,a} x^a e^{\tau \omega_k(a)}.
\]
In practice, the path tracking process start from some \(t_0 < 0\) with sufficiently large magnitude. We refer to Refs. \[11, 15\] for detailed descriptions. The downside\[1\] is the potentially longer path parameter interval \([t_0,0]\). However, this technique is adopted by several polyhedral homotopy implementations \[3, 11, 15\] and the consensus is that the numerical benefits far outweighs the cost.

2.2. Projective formulation. Another issue one has to deal with is the existence of divergent paths, especially paths along which \(\|x\| \to \infty\) or grow very large. This is usually dealt with by lifting \(2\) into the complex projective space \(\mathbb{P}^n\). Using \(y = (y_0, y_1, \ldots, y_n)\) that represents homogeneous coordinates in \(\mathbb{P}^n\), \(2\) may be further reformulated as \(H^\text{hom} : \mathbb{C}^{n+1} \times (-\infty,0]\) with
\[
(3) \quad h_k^\text{hom}(y,\tau) = \sum_{a \in S_k} c_{k,a} y^{a\text{hom}} e^{\tau \omega_k(a)}, \quad \text{for} \ k = 1, \ldots, n,
\]
where \(a^\text{hom} = (a, \deg(f_i) - 1^\top a)^\top \in \mathbb{Z}^{n+1}\), for each \(a \in S_k \subset \mathbb{Z}^n\), represent the exponent vectors of the corresponding monomials in the homogenization of \(f_k\). Then \(H^\text{hom} = (h_1^\text{hom}, \ldots, h_n^\text{hom})\) is homogeneous in \(y\), and represents the lifting of the homotopy \(2\) into the complex projective space. We refer to Refs. \[1, 2, 17, 19\] for discussions on this topic.

\[1\]Another apparent downside is the use of potentially expensive exponential function. However, the original formulation \(1\) already requires the computation of rational powers \(t^{-\omega_k(a)}\), which are computed indirectly via exponential functions, so the use of exponential functions is unavoidable in most practical implementations.
2.3. Euler and Newton directions in path tracking. In the affine formulation [2], the paths in \((\mathbb{C}^*)^n \times (-\infty, 0]\) are defined by \(H(x, \tau) = 0\). Along each, by the Implicit Function Theorem, \(x\) is a smooth function of \(\tau\), and \(\frac{dx}{d\tau}\), as a column vector, is characterized by the Davidenko equation

\[
\frac{\partial H}{\partial x}(x, \tau) \frac{dx}{d\tau}(x, \tau) + \frac{\partial H}{\partial \tau}(x, \tau) = 0.
\]

This vector shall be referred to as the Euler direction in affine coordinates of a solution path at a given point on the path, and we shall use the notation \(E(x, \tau) := \frac{dx}{d\tau}(x, \tau)\).

The corresponding Euler direction \(E(y, \tau)\) in homogeneous coordinates is characterized by

\[
\frac{\partial H^\text{hom}}{\partial y}(y, \tau) E(y, \tau) + \frac{\partial H^\text{hom}}{\partial \tau}(y, \tau) = 0,
\]

and

\(y^* E(y, \tau) = 0\),

where \(y^*\) is the row vector whose entries are the conjugates of the entries of \(y\). \(E(y, \tau)\) represents the geodesic direction defined by the path with respect to the Fubini-Study metric on \(\mathbb{P}^n\). We again refer to Ref. [7] for the derivation.

The name, “Euler direction” refers to the fact that in both form, \(\Delta \tau \mapsto x(\tau) + \Delta \tau E(x, \tau)\) and \(\Delta \tau \mapsto y(\tau) + \Delta \tau E(y, \tau)\) are the first order approximations of the solution path provided by the Euler’s method, in the affine and homogeneous coordinates, respectively. Under the smoothness assumption, both are uniquely defined. They can be used in any predictor methods that utilize first order derivative information. In particular, they are directly used in Euler’s method, Cubic Hermite method, and certain spline-based methods. They are also indirectly used in predictors based on Runge-Kutta (Runge-Kutta-Fehlberg) methods.

Similarly, the Newton direction, in affine coordinates, is the unique vector \(N(x, \tau)\) such that

\[
\frac{\partial H}{\partial x}(x, \tau) N(x, \tau) + H(x, \tau) = 0,
\]

and the corresponding Newton direction in homogeneous coordinates, \(N(y, \tau)\) is defined by

\[
\frac{\partial H^\text{hom}}{\partial y}(y, \tau) N(y, \tau) + \frac{\partial H^\text{hom}}{\partial \tau}(y, \tau) = 0.
\]

They are vectors used in standard and projective Newton \([4][17]\) iterations respectively. The affine version can also be used in dampened Newton iterations and local Newton homotopy method.

3. Hardware architectures and the problem statement

Homotopy continuation methods, including the polyhedral homotopy described above, are naturally parallel and scalable in the sense that every solution can be computed independently (pleasantly parallel). The problem of implementing such parallel homotopy-based solvers on traditional computer clusters and multi-core CPU architectures has been thoroughly explored. However, today, the landscape of high performance computing is dominated by GPUs (graphical processing units), and the same type of algorithms cannot be ported directly to modern GPUs with the same level of efficiency and scalability due to the inherent hardware constraints: At the lowest level, modern GPUs gain their superiority in computational power from their single-instruction-multiple-data (or SIMD) architecture, in which multiple processing unit perform the exact same mathematical operation on multiple data points simultaneously. Newest CPUs also support SIMD models (e.g., through Intel’s AVX instructions) to a certain extend. Such architectures exploit data-parallelism, but not true concurrency, hence the limitations.

Single-instruction-multiple-threads (or SIMT) is a subclass of SIMD in Flynn’s 1972 taxonomy [9]. It is loosely defined by the parallel computing units having their own independent registers and memory (cache and data Memory), which better describes the higher level data organization
in modern GPUs. We will also include the structurally similar Tensor Cores\(^2\) in our target model. Tensor cores specialize in general matrix multiplications (GEMM), which also resembles a SIMT model from an algorithmic point of view. To target these hardware devices, we assume a heterogeneous memory model in which threads have access to different memory types with different latency and bandwidth expectations.\(^3\)

For simplicity, the hardware architectures with all these constraints, including GPUs, CPU with AVX instruction sets, and the new tensor cores will simply be referred to as the SIMD/SIMT architecture. The computational framework proposed in this paper directly targets such a SIMD/SIMT architecture and only this architecture.

The central problem here is to...

(1) evaluate \(H\) and its Jacobian matrix (i.e., all its partial derivatives) simultaneously, and (2) compute the Euler and Newton directions simultaneously, while optimizing the algorithm subject to the constraints of the SIMD/SIMT hardware architecture. In particular, the algorithm must...

(a) minimize data transfer, (b) minimize global memory access, (c) minimize communication between devices, and (d) extract parallelism from multiple levels (e.g., monomial, variable, path, and hardware level).

In Sections 5 and 6 we propose a simple algorithm that solve this problem under the given hardware constraints.

4. Related works

Evaluating multivariate systems together with their Jacobian matrices efficiently is a basic problem in numerical computation (see, e.g., Ref. [5]). In the context of homotopy continuation methods, this problem was analyzed rigorously in Ref. [13] through the framework of multivariate generalization of the Horner’s rule. Several algorithms have been designed specifically for GPUs [20, 21]. Several algorithms originally designed for CPUs [6, 15] have also been ported to CUDA-based GPUs.

One distinguishing feature of the algorithm proposed in this paper is its stark simplicity. More importantly, the proposed approach formulates the central problem into problems that GPUs are optimized — “BLAS operations” [3, 14].

5. Formulating homotopy evaluation as matrix multiplication

5.1. Logarithmic formulation. For simplicity, we assume the target system \(F = (f_1, \ldots, f_n)\) to be “unmixed”, i.e., the support of \(f_1, \ldots, f_n\) are identical. We also restrict ourselves to solutions within \((\mathbb{C}^*)^n\) like the original polyhedral homotopy formulation. Under these assumptions, we formulate the problem of evaluating the homotopy function \(H^{\text{hom}}\), in [3] together with all its partial derivatives as a problem of general matrix multiplication (GEMM), which maps nice to the SIMD/SIMT architectures.

We first lift \(H\) into the logarithmic coordinate space. Fixing any branch \(\log : \mathbb{C}^* \to \mathbb{C}\) of the complex logarithm function, we introduce new variables \(z = (z_0, \ldots, z_n)\) through the relations

\[
(6) \quad y = \log \begin{pmatrix} y_0 \\ \vdots \\ y_n \end{pmatrix} = \log \begin{pmatrix} z_0 \\ \vdots \\ z_n \end{pmatrix}.
\]
Though this depends on the choice of the branch of log, the projection $y = e^x = (e^{z_1}, \ldots, e^{z_n})$ remains valid and well-defined regardless of the choices. Thus, under the restriction $y \in (\mathbb{C}^*)^n$, this represents a locally smooth change of variables. Under the “unmixed” assumption, we define $S := \{a_1, \ldots, a_m\} = S_1 = \cdots = S_n$ to be the common support of $f_1, \ldots, f_n$, and let $\{\omega_1, \ldots, \omega_m\}$ be the corresponding lifting values. We also use the notations

$$N = n + 1$$

$$\hat{z} = (z, \tau),$$

$$\hat{a}_k^\text{hom} = (a_k^\text{hom}, \omega_k)\top \quad \text{for } k = 1, \ldots, m,$$

$$\hat{A}^\text{hom} = [\hat{a}_1^\text{hom} \quad \cdots \quad \hat{a}_m^\text{hom}] \in M_{(N+1)\times m}(\mathbb{Z}).$$

Then the collection of monomials in $h_k^\text{hom}(y, \tau)$, as a row vector, can be expressed as

$$y^{a_1^\text{hom}} e^{\tau \omega_1} \cdots y^{a_m^\text{hom}} e^{\tau \omega_m} = \begin{bmatrix} e^{\langle \hat{z}, \hat{a}_1^\text{hom} \rangle} & \cdots & e^{\langle \hat{z}, \hat{a}_m^\text{hom} \rangle} \end{bmatrix} = e^{\hat{z} \hat{A}^\text{hom}}$$

This leads to the compact expression

$$h_k^\text{hom}(y, \tau) = e^{\hat{z} \hat{A}^\text{hom}} \cdot c_k \quad \text{for } k = 1, \ldots, n$$

where $c_k = (c_{k,1}, \ldots, c_{k,m})\top$ is the column vector that collects the coefficients of the terms in $h_k^\text{hom}$ for $k = 1, \ldots, n$.

The logarithmic coordinate turns the computation of monomials into a simple vector-matrix product $\hat{z} \mapsto \hat{z} \hat{A}^\text{hom}$, which is particularly efficient to compute on SIMD/SIMT architectures. However, the true benefit of the formulation \[S\] is the ease with which partial derivatives can be computed using existing data. In particular,

$$\frac{\partial h_k^\text{hom}}{\partial z_j} = \frac{\partial}{\partial z_j} \left(e^{\hat{z} \hat{A}^\text{hom}} \cdot c_k\right) = e^{\hat{z} \hat{A}^\text{hom}} \cdot \begin{bmatrix} c_{k,1}^{a_1^\text{hom}} \\ \vdots \\ c_{k,m}^{a_m^\text{hom}} \end{bmatrix} \quad \text{for } j = 0, \ldots, n.$$  

Notice that the vector appeared at the end is precisely the entrywise product (Hadamard product) between the coefficient vector $c_k$ and the transpose of the $j$-th row of $\hat{A}^\text{hom}$. To further simplify the notation as well as the data organization, we define $(N + 2) \times m$ matrices

$$B_k = \begin{bmatrix} c_{k,1}^{a_1^\text{hom}} & \cdots & c_{k,m}^{a_m^\text{hom}} \\ c_{k,1}^\top & \cdots & c_{k,m}^\top \end{bmatrix}, \quad \text{for } k = 1, \ldots, n,$$

which will remain constant and thus can be pre-computed prior to the path tracking process. Then, for any $k = 1, \ldots, n$, the function value $h_k^\text{hom}$ and all its partial derivatives with respect to $(z_0, \ldots, z_n, \tau)$ and $(y_0, \ldots, y_n, \tau)$ can be computed as the row vectors

$$\begin{bmatrix} \partial h_k^\text{hom} \\ D_z h_k^\text{hom} \end{bmatrix} = \begin{bmatrix} \partial h_k^\text{hom} \\ \vdots \\ \partial h_k^\text{hom} \end{bmatrix}, \quad \text{and} \quad \begin{bmatrix} \partial h_k^\text{hom} \\ D_{\tau} h_k^\text{hom} \end{bmatrix} = \begin{bmatrix} \partial h_k^\text{hom} \\ \vdots \\ \partial h_k^\text{hom} \end{bmatrix} h_k^\text{hom} = e^{\hat{z} \hat{A}^\text{hom}} B_k^\top, \quad \text{for } k = 1, \ldots, n.$$  

To apply these formulations to all components of $H^\text{hom}$, it is convenient to define the extended Jacobian matrices in logarithmic and homogeneous coordinates to be

$$\hat{D}_z H^\text{hom} := [D_z H^\text{hom} \quad D_{\tau} H^\text{hom} \quad H^\text{hom}] \quad \text{and} \quad \hat{D}_y H^\text{hom} := [D_y H^\text{hom} \quad D_{\tau} H^\text{hom} \quad H^\text{hom}].$$

Then the vectorization of these matrices can be computed as

$$\text{vec}(\hat{D}_z H^\text{hom}) = e^{\hat{z} \hat{A}} \begin{bmatrix} B_1^\top & \cdots & B_n^\top \end{bmatrix}$$

$$\text{vec}(\hat{D}_y H^\text{hom}) = e^{\hat{z} \hat{A}} \begin{bmatrix} B_1^\top \text{diag}(e^{-z}, 1, 1) & \cdots & B_n^\top \text{diag}(e^{-z}, 1, 1) \end{bmatrix}.$$
5.2. Batched evaluation at a large number of points. The main advantage of SIMD/SIMT architectures, such as GPU devices, is their ability in carrying out identical and independent operations on large sets of data at the same time. Indeed, operating on sufficiently large data set is the main mechanism by which latency can be hidden. This characteristic maps well to the path tracking problem due to its “pleasantly parallel” nature.

For \( p \) different points \( \hat{z}_1, \ldots, \hat{z}_p \) in \( \mathbb{C}^{n+1} \) with \( \hat{z}_k = (z_k, \tau_k) \), the vectorization of the extended Jacobian matrix \( \hat{D}_z H^{\text{hom}} \) evaluated at these points can thus be computed simultaneously as

\[
\begin{bmatrix}
\text{vec}(\hat{D}_z H^{\text{hom}}(\hat{z}_1)) \\
\vdots \\
\text{vec}(\hat{D}_z H^{\text{hom}}(\hat{z}_p))
\end{bmatrix} = e^{\hat{Z} \hat{A}} [B_1^\top \cdots B_n^\top]
\]

where \( \hat{Z} = \begin{bmatrix} \hat{z}_1 \\
\vdots \\
\hat{z}_p \end{bmatrix} \), and, with a slight abuse of notations, we consider \( e^{\hat{Z} \hat{A}} \) to be a \( p \times m \) matrix whose \( k \)-th row is \( e^{\hat{z}_k \hat{A}} \). Its counterpart in homogeneous coordinate can be computed from the above formula by multiplying \( \text{diag}(e^{-\hat{z}_i}, 1, 1) \) to each block.

The simultaneous evaluation of \( H^{\text{hom}} \) and all its partial derivatives, i.e., the extended Jacobian matrix, at a large number of points is thus formulated as a general matrix multiplication (GEMM) operation (a level-3 BLAS operation), which is one of the operations GPUs (especially tensor cores) are optimized to carry out. When the number of points \( p \) is sufficiently large, this operation can hide latency effectively.

6. Simultaneous computation of the Euler and the Newton direction

We extract an additional level of parallelism from the simultaneous computation of the Euler and Newton direction through a single unified process. Even though the two directions are rarely used together, this design consolidates the two independent steps, which eliminates the costs associated with synchronizations and greatly simplifies the data pathways. More importantly, it eliminates complicated branching (i.e., high level decision-making) from the GPU side.

To take full advantage of the SIMD/SIMT architecture, one must leverage of the benefit of “batched” operations, i.e., structurally identical matrix operations applied to a large number of matrices of the same size and memory layout. Not all matrix operations can be consolidated into batch mode, and thus the operations must be chosen with care.

Recall that the Euler direction \( E(y, \tau) \) and the Newton direction \( N(y, \tau) \) are defined by the nonsingular linear systems

\[
\begin{align*}
\frac{\partial H^{\text{hom}}}{\partial y} E(y, \tau) + \frac{\partial H^{\text{hom}}}{\partial \tau} = 0, & \quad \text{and} \quad y^* \frac{dy}{d\tau} = 0; \\
\frac{\partial H^{\text{hom}}}{\partial y} N(y, \tau) + H^{\text{hom}} = 0, & \quad \text{and} \quad y^* \Delta y = 0.
\end{align*}
\]

The similarity between the two suggests that the equations can be unified into the system

\[
(11) \quad \begin{bmatrix}
\frac{\partial H^{\text{hom}}}{\partial y} & \frac{\partial H^{\text{hom}}}{\partial \tau} \\
y^* & 0
\end{bmatrix} \begin{bmatrix}
\frac{dv}{d\tau} \\
\Delta y
\end{bmatrix} = 0.
\]

Note that the matrix on the left contains the extended Jacobian matrix \( \hat{D}_y H^{\text{hom}} \). Therefore, they can be computed through a numerically stable QR decomposition. After finding an \((N+2) \times (N+2)\) unitary matrix \( Q \) and an \( N \times N \) upper triangular matrix \( R \) such that

\[
J^\top := \begin{bmatrix}
\frac{\partial H^{\text{hom}}}{\partial y} & \frac{\partial H^{\text{hom}}}{\partial \tau} \\
y^* & 0
\end{bmatrix} = Q \begin{bmatrix}
R \\
0_{2 \times n}
\end{bmatrix},
\]

\[
\begin{bmatrix}
\frac{dv}{d\tau} \\
\Delta y
\end{bmatrix} = R^{-1} \begin{bmatrix}
\Delta y
\end{bmatrix}.
\]
then the null space of $J$ is spanned by the two vectors $(e_{N+1}Q^*)^\top$ and $(e_{N+2}Q^*)^\top$, i.e., the complex conjugate of the right most two columns of $Q$. After further reduction, the Euler and Newton directions are computed.

If we further assume $\hat{D}_y H^\hom$ to be well conditioned, then this process can be carried out via simple Householder transformations, which, on most modern SIMD/SIMT architectures, can be process in “batch mode” on a large number of points simultaneously.

**Remark 1.** In particular, on NVIDIA CUDA architecture, this can be achieved through “batched QR-decomposition” offered by cuBLAS library.

**Remark 2.** If $\hat{D}_y H^\hom$ is ill-conditioned, more advanced QR decomposition methods have to be used. Currently, these are not supported by the standard NVIDIA CUDA framework. One potential solution is to use more advance solver libraries such as MAGMA. Alternatively, pre-conditioners can be used to improve the numerical conditions of $\hat{D}_y H^\hom$ prior to this step. The pros and cons of these solutions will be investigated in future studies.

7. **Summary of the algorithm**

In the following, we summarize the main algorithms and provide pseudocode for an implementation targeting GPUs. We assume the target GPU has heterogeneous memory organization, i.e., there is a distinction between “host” (CPU) memory and “device” (GPU) memory, and transferring data between the two is slow and must be minimized. Operations in pseudocode will be marked by “(Host)”, “(Device)”, or “(Host→device)” to indicate if an operation access host memory, device memory, or transfer data from host memory to device memory. There is also a nonhomogeneous hierarchy of different device memory types. Their distinctions are left as implementation details and not directly described here.

Algorithm 1 allocate device memory and initialize constant matrices to be used in later computations. Here $p \in \mathbb{Z}^n$ is the maximum number of points, i.e., paths, to be stored simultaneously on a GPU device. This number is mainly limited by the available global memory on device.

**Algorithm 1** Initialization procedure

1: procedure Initialize($p, c_1, \ldots, c_n, \hat{A}^\hom$)
2: (Host→device) Transfer coefficient vectors $c_1, \ldots, c_n$ to device;
3: (Host→device) Transfer exponent matrix $\hat{A}^\hom$ to device;
4: (Device) Allocate $p \times (N + 1)$ $\mathbb{C}$-matrix for $\hat{Z}$;
5: (Device) Allocate $p \times (N + 1)$ $\mathbb{C}$-matrix for $\hat{Y}$;
6: (Device) Allocate $p(n + 1) \times (N + 2)$ $\mathbb{C}$-matrix for $J$;
7: (Device) Allocate $(N + 1) \times m$ $\mathbb{C}$-matrix for $B_k$ for each $k = 1, \ldots, n$;
8: (Device) Allocate $2p \times (N + 2)$ $\mathbb{C}$-matrix for $V_i$ for each $i = 1, \ldots, n$;
9: (Device) $B_k \leftarrow \begin{bmatrix} \hat{A}^\hom \text{diag}(c_k) \\ c_k \end{bmatrix}$ for $k = 1, \ldots, n$;
10: end procedure

To hide latency, the evaluations of the extended Jacobian matrices are carried out in batches. The $p$ points $\hat{y}_1, \ldots, \hat{y}_p$ are divided into batches of some given size $b$. For the $i$-th batch, Algorithm 2 evaluates the extended Jacobian matrices $\hat{D}_y \hat{H}^\hom(\hat{y}_k)$ for $k = ib + 1, \ldots, ib + b$. In it, $Z_{i,b}$ and $Y_{i,b}$ are the submatrices of $Z$ and $Y$, respectively, corresponding to the $i$-th batch of points. The results are stored in the corresponding submatrix $J_{i,b}$ in $J$. The evaluation for multiple batches are carried out concurrently, so that operation 2 of Algorithm 2 is applied to one batch of points while the result of operation 3 for the previous batch is being written to device global memory, thereby
Algorithm 2 Batched evaluation of extended Jacobian matrix

1: procedure EVALUATE($i, b$)
2:  (Device) $Z_{i,b} \leftarrow \log(Y_{i,b})$;
3:  (Device) $J_{i,b} \leftarrow e^{Z_{i,b}}[B_1^\top \cdots B_n^\top]$;
4:  (Device) Multiply $\text{diag}(e^{-z_i}, 1, 1)$ to the $i$-th block of $J$ for $i = 1, \ldots, p$;
5: end procedure

Effectively hiding latency. The optimal batch size $b$ is dependent on specific hardware characteristics (e.g. the relative speed at which the target GPU can carry out computational-intensive tasks vs memory-intensive tasks).

Algorithm 3 Computation of Euler and Newton directions

1: procedure EULERNEWTON($i, b$)
2:  (Device) Compute the pointer of $\hat{D}_y H_{\text{hom}}(y_i)$ within $J$;
3:  (Device) Compute the QR decomposition of $\hat{D}_y H_{\text{hom}}(y_i)^\top = Q_i \begin{bmatrix} R_i \\ 0_{2 \times n} \end{bmatrix}$;
4:  (Device) $V_i \leftarrow \begin{bmatrix} e_{N+1} \\ e_{N+2} \end{bmatrix} Q_i^*$;
5:  (Device) Perform row reduction so that rightmost $2 \times 2$ block of $V_i$ is $I$.
6: end procedure

The Euler and Newton directions are computed by Algorithm 3. The results, as $2 \times N$ matrices are stored in the leftmost columns of $V_i$'s, which reside in device (global) memory.

8. Preliminary implementation and experiments

As a proof of concept, the main algorithms are implemented through CUDA framework and supports NVIDIA's general-purpose GPUs (GPGPUs). In particular, it relies on the cuBLAS library for efficient usage of GPU resource.

In the base implementation, the general matrix multiplication (GEMM) operations is carried out by the function `cublasZgemm`, which performs complex matrix multiplications in double precision. The QR decomposition computation, in Algorithm 3 operation 3, is carried out by the function `cublasZgeqrfBatched`, which automatically schedules the decomposition of a large number of matrices and effectively hiding latency.

In the variant that supports tensor core operations, Algorithm 2 (specifically operation 3 of Algorithm 2) runs on tensor cores with much greater efficiency. In that case, since Algorithm 3 runs on CUDA cores, in principle, these two algorithms can run concurrently on different batches of points.

Table 1 shows tests of this experimental implementation on the well known “cyclic-14” system, which is a system of 14 polynomial equations in 14 (complex) variables with a total of 184 distinct monomials. Mobile (notebook computer) GPU NVIDIA Quadro T2000, NVIDIA Tesla K80 (released in 2014), and NVIDIA V100 (released in 2017) are used in these testings. The results represent the

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4Only recent GPUs of “Pascal” micro-architecture or newer are directly supported due to the use of newer features. Tensor core features are only supported on NVIDIA A100 and A30 that have double precision tensor cores.

5Even though NVIDIA’s GPUs for high performance computing starting from V100, release in 2017, all support tensor cores, only the more recent A100 and A30 directly support double precision computation on tensor cores. As a result, tensor core operations are disabled for GPUs older than A100 and A30.

6Tesla K80 contains two GPUs, only one of them is used in all the testings.
average of 3 different runs. To keep the test results consistent, a simplified “Euler-Newton” step is used, in which a single Euler prediction step is followed by a single Newton iteration. In all runs, the batch size is set to $\frac{1}{4}p$, where $p$ is the number of points to be processed simultaneously. This is likely far from optimal for hiding latency. Further testing and analysis are needed to determine the optimal batch size. Similarly, Table 2 shows the test results on the Chandra-24 system, which is a system of 24 polynomial equations in 24 (complex) variables with a total of 324 distinct monomials. Both tests suggest the very promising scalability of this GPU-accelerated approach. In particular, the timing information on NVIDIA V100 GPU appear to be constant regardless the number of points are processed. This indicates that the computational time (latency) is still dominated by host-device memory transfer and other memory-bound operations, and thus the algorithm can scale even further if memory transfer can be optimized or reduced.

| GPU          | Mobile GPU Quadro T2000 | Tesla K80 | V100 |
|--------------|-------------------------|-----------|------|
| 10 points    | 0.0744s                 | 0.0850s   | 0.0222s |
| 50 points    | 0.0888s                 | 0.0991s   | 0.0274s |
| 250 points   | 0.1910s                 | 0.1092s   | 0.0296s |
| 500 points   | 0.3330s                 | 0.2059s   | 0.0313s |
| 1000 points  | 0.7035s                 | 0.4120s   | 0.0355s |

Table 1. Wall-clock time, in seconds, for performing 100 consecutive Euler-Newton steps for the cyclic-14 system on groups of points of different sizes using various NVIDIA GPUs.

| GPU          | Mobile GPU Quadro T2000 | Tesla K80 | V100 |
|--------------|-------------------------|-----------|------|
| 250 points   | 0.8219s                 | 0.3266s   | 0.0728s |
| 500 points   | 1.7084s                 | 0.6461s   | 0.0757s |
| 1000 points  | -                       | 1.1902s   | 0.0852s |

Table 2. Wall-clock time, in seconds, for performing 100 consecutive Euler-Newton steps for the chandra-24 system on groups of points of different sizes using various NVIDIA GPUs. “-” indicate the test cannot be completed as a single run due to GPU memory limitation.

For a comparison with existing CPU-based algorithms, we choose the implementation in Hom4PS-3 which adopts the basic algorithm in HOM4PS-2.0. Moreover, using Intel MKL (math kernel library), the BLAS-based algorithm proposed here can also be easily ported back to modern CPU that support AVX-512 instructions. Intel MKL also supports older CPUs that do not support AVX-512 instructions. However, in those cases, hardware acceleration may have minimum effect.

7In actual path trackers, the number of Newton iterations depends on the quality of the prediction. Here, we fix the number of iterations to be exactly 1 so that the timing information from different runs can be compared.

8Best efforts are made to keep the comparisons fair. However, the implementation in Hom4PS-3 is fundamentally different as additional steps are carried out to store information for higher order predictor-corrector algorithms. It appears the time consumed by these additional steps is small in comparison.

9Intel MKL also supports older CPUs that do not support AVX-512 instructions. However, in those cases, hardware acceleration may have minimum effect.
(1) The proposed GPU-accelerated algorithm;
(2) The proposed algorithm implemented on modern CPUs (restricted to a single core);
(3) The proposed algorithm implemented on modern CPUs (using 8 cores);
(4) The existing Hom4PS-3 (CPU-only) algorithm.

The result shows the clear advantage of the GPU-accelerated algorithm as the proof-of-concept implementation is already showing vastly superior performance and scalability. Interestingly, even when ported back to CPUs (using Intel MKL), the proposed algorithm still appear to be faster than the existing implementation in Hom4PS-3.

| Algorithm                      | GPU version of the proposed algorithm based on CUDA | CPU version of the same algorithm using BLAS on 1 core | CPU version of the same algorithm using BLAS on 8 cores | Hom4PS-2/3 algorithm running on 8 cores |
|-------------------------------|--------------------------------------------------|-----------------------------------------------------|-----------------------------------------------------|--------------------------------------|
| Time                          | 0.0852s                                           | 10.7149s                                             | 1.3901s                                             | 3.3090s                              |

Table 3. Wall-clock time, in seconds, for performing 100 consecutive Euler-Newton steps for the chandra-24 system on a group of 1000 points on GPU (NVIDIA V100) and CPU (Intel Xeon E5-2686 v4) using different algorithms.

9. Concluding remarks

We proposed an extremely simple approach for efficiently evaluating a homotopy function together with all its partial derivatives, in the context of the polyhedral homotopy method of Huber and Sturmfels, that maps particularly well to modern GPUs (and similar hardware architectures). This is done through a reformulation of the problem of evaluating Laurent polynomial systems together with their derivatives into general matrix multiplication (GEMM) operations. Based on this, we also proposed a companion algorithm that unifies the computation of Euler and Newton directions which are needed in path tracking. Together, they allow the entire path tracking process to be carried out by GPUs.

Our experimental implementation shows promising efficiency and scalability when compared to existing CPU-based algorithms. Further optimizations are needed to realize the full potential of this approach. In particular, minimizing host-device communication, optimizing memory layout, and properly hiding latency appear to be the most important tasks.

In the experimental implementation, no effort was made to analyze and improve the accuracy, stability, and numerical condition of evaluation of the homotopy function together with its partial derivatives. The necessity and design of pre-conditioners for ensuring the numerical quality of this step will also be a crucial task in future studies.

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