Accelerating Optimal Power Flow with GPUs: SIMD Abstraction of Nonlinear Programs and Condensed-Space Interior-Point Methods

Sungho Shin and Mihai Anitescu
Mathematics and Computer Science Division
Argonne National Laboratory
Lemont, IL, USA
sshin@anl.gov, anitescu@mcs.anl.gov

François Pacaud Centre Automatique et Systèmes Mines Paris - PSL Paris, France francois.pacaud@minesparis.psl.eu

Abstract—This paper introduces a novel computational framework for efficiently solving AC optimal power flow (OPF) problems using GPUs. Although GPUs have demonstrated remarkable performance in various computing domains, their application in AC OPF has been limited due to challenges such as serial computations for automatic differentiation (AD) and sparse matrix factorization. To address these obstacles, we propose two strategies. First, we utilize a single-instruction, multiple-data (SIMD) abstraction of nonlinear programs (NLP). This approach allows us to specify model equations while preserving their parallelizable structure. By implementing AD on GPUs efficiently, we can fully leverage the computational power of these devices. Second, we employ a Condensed-Space Interior-Point Method (IPM) with inequality relaxation. This technique involves relaxing equality constraints to inequalities and condensing the Karush-Kuhn-Tucker system to the primal space. As a result, we enable efficient sparse matrix factorization on GPUs without requiring a numerical pivoting procedure. By combining these strategies, we achieve efficient AC OPF problem solutions on GPUs, keeping the problem data residing in the device memory and performing the majority of computations on the GPUs. Comprehensive numerical benchmark results showcase the substantial computational advantage of our approaches for solving AC OPF problems up to moderate precision on NVIDIA GPUs. Remarkably, our method achieves an order of magnitude speedup compared to state-of-theart tools on CPUs, such as JuMP.jl, AMPL, and Ipopt. The paper concludes by discussing the future extensibility of our method.

I. Introduction

While graphics processing units (GPUs) have demonstrated remarkable capabilities in various computing domains, their adoption in large-scale constrained nonlinear optimization regimes, such as alternating current (AC) optimal power flow (OPF) problems, has faced some limitations. One of the primary challenges arises from the automatic differentiation (AD) of sparse model equations and the parallel factorization of indefinite sparse matrices commonly encountered within constrained optimization algorithms [1]. While GPU computation can trivially accelerate several parts of the optimization process, especially various internal computations within the optimization solver, the sluggish data transfer between host and device memory hampers the ad-hoc implementation of GPU accelerations (Fig. II-C). To fully leverage the potential

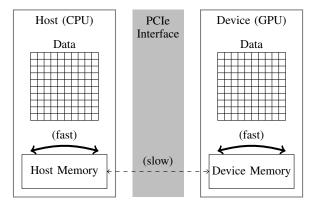


Fig. 1. A schematic description of host (CPU) and device (GPU) memory.

that modern GPU hardware has to offer, it becomes imperative to have a comprehensive computational framework for optimization on GPUs so that AD, linear algebra operations, and optimization can be performed entirely on the GPU. Specifically, for best performance, both the problem data and the solver's intermediate computational data must be exclusively resident within the device memory, with the majority of operations executed on the GPU.

This paper presents our approach to implement a comprehensive computational framework for solving large-scale OPF problems on NVIDIA GPUs, along with the associated software implementations: SIMDiff.jl, an AD tool, and MadNLP.jl, a nonlinear optimizaiton solver. Our approach incorporates two novel strategies: (i) a single-instruction, multiple-data (SIMD) abstraction of nonlinear programs (NLPs), enabling streamlined parallel AD on GPUs, and (ii) a condensed-space interior-point method (IPM) with an inequality relaxation strategy, which facilitates the use of highly efficient *refactorization* routines for sparse matrix factorization with fixed pivot sequences.

While derivative evaluation can be generally cheaper than linear algebra operations, our numerical results show that AD often constitutes more than half of the total solver time when using off-the-shelf AD implementations like JuMP.jl

or AMPL. Instead of the general-purpose tools, our method leverages a specialized AD implementation based on the SIMD abstraction of NLPs. This abstraction alllows to preserve the parallelizable structure within the model equations, facilitating efficient derivative evaluations on the GPU. The AC power flow model is particularly well-suited for this abstraction as it involves repetitive expressions for each component type (e.g., buses, lines, generators), and the number of computational patterns does not increase with the network's size. Numerical results reported in this paper demonstrate that our proposed strategies can achieve over 20 times speedup. In comparison to general AD implementations on CPUs (such as AMPL and JuMP.jl), our GPU-based method is approximately 50 times faster in the largest instances.

Linear algebra operations, especially sparse indefinite matrix factorization, are typically the bottleneck in nonlinear optimization solvers. Parallelizing this operation is challenging due to the need for numerical pivoting, which ensures the numerical stability. However, when the matrix can be factorized without numerical pivoting, a significant part of the operation can be parallelized, and the numerical factorization can be efficiently performed on GPUs. We develop a condensed-space IPM strategy that allows the use of sparse matrix factorization routines without numerical pivoting. This strategy relaxes equality constraints by permitting small violations, which enables expressing the Karush-Kuhn-Tucker (KKT) system entirely in the primal space through the condensation procedure. Although this strategy is not new [2], it has traditionally been considered less efficient than the standard full-space method due to increased nonzero entries in the KKT system. However, when implemented on GPUs, it offers the key advantage of ensuring positive definiteness in the condensed KKT system through the application of standard regularization techniques. This, in turn, allows for the utilization of linear solvers with a fixed numerical pivot sequence (known as refactorization). An efficient implementation of sparse refactorization is available as part of the CUDA library, enabling the implementation of efficient KKT system solutions on GPUs. Although this method is susceptible to numerical stability issues due to increased condition number in the KKT system, our results demonstrate that the solver is robust enough to solve problems with a relative accuracy of $\epsilon_{\rm mach}^{1/4}\approx 10^{-4}$.

We present numerical benchmark results to showcase the efficiency of our proposed approach, utilizing two of our packages: MadNLP.jl and SIMDiff.jl. The solution of the KKT system is performed using the external cuSOLVER library. To assess the performance of our method, we compare it against standard CPU approaches using the widely used data available in pglib-opf [3]. Our benchmark results demonstrate that our proposed computational framework has significant potential for accelerating the solution of AC OPF problems, particularly for large-scale instances, especially when a moderate tolerance (e.g., 10⁻⁴) is considered. Specifically, when running on NVIDIA GPUs, our method achieves a notable 4x speedup compared to our solver running on CPU, in the case of the largest instance. Moreover for the same instance, our approach

surpasses the performance of existing tools (such as Ipopt interfaced with JuMP,jl) by an order of magnitude. This finding underscores the importance of harnessing the computational power of GPUs as a key enabler for tackling the challenges posed by large-scale OPF problems.

Organization: The paper is organized as follows. In the remainder of the current section, we introduce the mathematical notation. In Section II, we provide general preliminary knowledge on numerical optimization and GPU computing. In Section III, we present the SIMD abstraction strategy for large-scale nonlinear programs and their advantages in terms of implementing parallel AD. Section IV presents the optimization algorithm under study, the condensed-space interior point method with inequality relaxation strategy. Section V presents the numerical results, comparing our approach with other state-of-the-art solution methods on GPUs. Finally, conclusions and future outlooks are given in Section VI.

Notation: We denote the set of real numbers and the set of integers by \mathbb{R} and \mathbb{I} . We let $[M] := \{1, 2, \cdots, M\}$. We let $[v_i]_{i \in [M]} := [v_1; v_2; \cdots, v_M]$. A vector of ones with an appropriate size is denoted by 1. We use the following convention for any symbol x: $X := \operatorname{diag}(x)$.

II. PRELIMINARIES

This section covers three essential background topics: numerical optimization, AD, and GPU computing.

A. Numerical Optimization

We consider NLPs of the form:

$$\min_{x^{\flat} \le x \le x^{\sharp}} f(x) \tag{1a}$$

s.t.
$$q(x) = 0$$
. (1b)

Numerous solution algorithms have been developed in the NLP literature. These methods can be broadly classified into active-set methods and interior-point methods [2]. Active-set methods aim to find the set of active consraints associated with the optimal solution in a combinatorial manner, while interior-point methods replace inequality constraints with smooth barrier functions, enabling the use of Newton-type second-order algorithms. Interior-point methods are known to be more scalable for problems with a large number of constraints and suitable for parallelization, thanks to the fixed sparsity pattern of the KKT matrix. We adopt the interior-point approach and develop our optimizationmethods on GPUs.

In terms of practical computations, three key components play vital roles: derivative evalutions (often provided by the AD capabilities of the algebraic modeling languages), linear algebra operations, and internal computations within the solver. Notably, most of the computational efforts are delegated to the external linear solver and AD library. The optimization solver orchestrates the operation of these tools to drive the solution iterate towards the stationary point of the optimization problem, but computations performed within the solver are generally much cheapr and simpler compared to the operations in AD and linear solver packages.

Since the successful implementation of the open-source interior point solver in Ipopt, many subsequent implementations of nonlinear optimization solvers [4], [5], [6] have been based on Ipopt [3]. We also use Ipopt as our main reference for the IPM implementation. Below, we outline the overall computational procedure employed wihtin nonlinear optimization frameworks:

- Given current primal-dual iterate $\begin{array}{lll} & (x^{(\ell)},y^{(\ell)},z^{\flat(\ell)},z^{\sharp(\ell)}), & \text{the} & \text{AD} & \text{package} & \text{computes:} \\ \nabla_x f(x^{(\ell)}), & \nabla_x g(x^{(\ell)}), & \nabla^2_{xx} \mathcal{L}(x^{(\ell)},y^{(\ell)},z^{\flat(\ell)},z^{\sharp(\ell)}), & \text{where} \\ \mathcal{L}(x^{\flat},y^{\flat},z^{\flat},z^{\flat}) := f(x) - y^{\top}g(x) - z^{\flat}(x-x^{\flat}) - z^{\sharp}(x^{\sharp}-x). \end{array}$
- 2) The following sparse indefinite system (known as the KKT system) is solved using sparse indefinite factorization (typically, via sparse LBL $^{\top}$ factorization) and triangular solve routines.

$$\begin{bmatrix} W^{(\ell)} + \Sigma^{(\ell)} + \delta_w^{(\ell)} I & A^{(\ell)\top} \\ A^{(\ell)} & -\delta_c I \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta y \end{bmatrix} = \begin{bmatrix} f - \mu X^{-1} \mathbf{1} \\ \Delta y \end{bmatrix}$$
(2)

Here, $W^{(\ell)} := \nabla^2_{xx} \mathcal{L}(x^{(\ell)}, y^{(\ell)}), \ A^{(\ell)} := \nabla_x g(x^{(\ell)}), \ \text{and}$ $\delta_w, \delta_c > 0$ are the regularization parameters determined based on the inertia correction procedure.

3) The optimization solver employs the filter line search procedure to determine the step size. While alternative approaches, such as trust-region-type methods and merit function-based criteria, can be used for determining the step size, the filter line search method is most commonly used due to its implementation in Ipopt.

B. AD

Efficiently evaluating the derivatives of $f(\cdot)$, $g(\cdot)$, and $\mathcal{L}(\cdot, \cdot)$ is crucial for the efficient solution of optimization problems.

Numerical differentiation of computer programs can be achieved through three different methods: (i) finite difference method, (ii) symbolic differentiation, and (iii) AD. The finite difference method suffers from numerical rounding errors, and its computational complexity grows unfavorably with respect to the number of function arguments, making it less preferable unless no other alternatives are available. Symbolic differentiation uses computer algebra systems to obtain symbolic expressions of first or higher-order derivatives. While this method can differentiate functions up to high numerical precision, it suffers from "expression swelling" effect and struggles to compute the derivatives of long nested expressions in a computationally efficient way.

In contrast, AD differentiates computer programs by leveraging the computation graph. By inspecting the computation graph and applying chain rules, AD can efficiently and accurately evaluate derivatives. This approach has become the dominant paradigm for derivative computation within the scientific computing domain, including nonlinear optimization and machine learning. For large-scale optimization, such as AC OPFs, AD tools are often implemented as part of domainspecific modeling languages, such as JuMP, CasADi, and AMPL (optimization) and Torch and Flux (machine learning).

There are two alternative ways of propagating derivatives through the recursive application of chain rules: (i) forwardmode and (ii) reverse-mode, which operate in opposite directions (from leaves to root and from root to leaves, respectively). Reverse-mode automatic differentiation, also known as an adjoint method, has proven to be particularly effective for dealing with the function expressions in large-scale optimization problems.

The Julia Language, our language of choice, provides convenient ways of implementing highly efficient automatic differentiation. Any Julia function, including commonly used operations such as addition, multiplication, trigonometric functions, exponential functions, and others, can be straightforwardly extended through the use of multiple dispatch paradigm, allowing functions to be dynamically dispatched based on the run-time type. Several implementations of AD are available in Julia, including ReverseDiff.jl, ForwardDiff.jl, Zygote.jl, and JuMP.jl. While these tools are general and useful for various applications, they are not optimized for evaluating derivatives of AC OPF problems, which contains an obvious parallelizable structure that can be exploited.

C. GPU Computing

With the increasing prevalence of GPU in various scientific computing tasks, there has been growing interest in leveraging these parallel systems to efficiently solve large-scale OPF problems. Some recent concurrent approaches include HyKKT, a hybrid (direct-iterative) KKT system solver, [7] and HiOP, a HPC solver for nonlinear optimization problems, [8]. However, adapting the IPM to GPUs presents challenges due to the fundamental differences between GPU and CPU programming paradigms. While CPUs execute a sequence of instructions on a single input (single instruction, single data, or SISD, in Flynn's taxonomy), GPUs run the same instruction simultaneously on hundreds of threads using the SIMD paradigm (see Fig. II-C). The SIMD parallelism works well for algorithms that can be decomposed into simple instructions running entirely in parallel, but not all algorithms seamlessly fit this paradigm. For example, branching in the control flow can hinder lockstep execution across multiple threads, and in turn, prevents efficient implementations on GPUs. On the other hand, when the algorithm's structure allows for efficient parallelization, the SIMD parallelism in GPUs becomes highly effective, and oftentimes enables orders of magnitudes speedup.

We highlight that the following, arguably quite common, computational patterns are particularly effective when implemented on GPUs:

$$y \leftarrow [g(x; q_j)]_{j \in [J]}$$
 (Pattern 1)

$$y \leftarrow y + \sum_{k \in [K]} h(x; s_k)$$
 (Pattern 2)
$$o \leftarrow \sum_{i \in [I]} f(x; p_i).$$
 (Pattern 3)

$$o \leftarrow \sum_{i \in [I]} f(x; p_i).$$
 (Pattern 3)

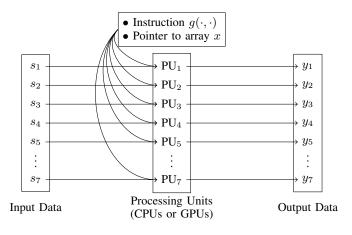


Fig. 2. A schematic description of SIMD parallelism in GPU computing

Here, it is assumed that $f: \mathbb{R}^{n_x} \times \mathbb{R}^{n_p} \to \mathbb{R}$, $g: \mathbb{R}^{n_x} \times \mathbb{R}^{n_s} \to \mathbb{R}$, and $h: \mathbb{R}^{n_x} \times \mathbb{R}^{n_p} \to \mathbb{R}^{n_y}$ are simple instructions that require only a handful of operations. Pattern 1 is typically most effective on GPUs, where each available thread can operate independently without needing to simultaneously manipulate the same data reference in device memory. Pattern 2 and Pattern 3 are more challenging to implement, as they require simultaneous access to the same device memory location, but they can be parallelized effectively by using buffers.

Many of the operations required in AD of sparse physical models, as well as the application of optimization algorithms, are based on the computational patterns mentioned above. For example, an OPF model can be implemented with 14 different computational patterns, all of which fall within the aforementioned categories. Additionally, the computation within optimization solvers, such as forming the left-hand-side for the KKT systems, computing the $\|\cdot\|_{\infty}$ norm of the constraint violation, and assembling the condensed KKT system, can be carried out by using these computational patterns. The only exception is the factorization of the sparse KKT matrix, which requires more sophisticated implementations.

Implementing kernel functions for the above computational patterns in the Julia Language is straightforward, as it provides excellent high-level interfaces for array and kernel programming for GPU arrays. The code can even be device-agnostic, thanks to the portable programming capability brought by KernelAbstractions.jl. All of the AD and optimization capabilities in our tools, MadNLP.jl and SIMDiff.jl, are implemented in Julia Language, utilizing its kernel and array programming capabilities.

III. SIMD ABSTRACTION OF NLPS

This section describes our implementation of SIMD abstraction and sparse AD of the model equations. The abstraction and AD are implemented as part of our algebriac modeling language SIMDiff.jl.

The SIMD abstraction under consideration is as follows:

$$\min_{x^L \leq x \leq x^U} \sum_{\ell \in [L]} \sum_{i \in [I_k]} f^{(\ell)}(x; p_i^{(\ell)}) \tag{3a} \label{eq:3a}$$

s.t.
$$\forall m \in [M]$$
: (3b)

$$g_{\flat}^{(m)} \leq \left[g^{(m)}(x;q_{j})\right]_{j \in [J]}$$

$$+ \sum_{n \in [N_{m}]} \sum_{k \in [K_{n}]} h^{(n)}(x;s_{k}^{(n)}) \leq g_{\sharp}^{(m)},$$
(3c)

where $f^{(\ell)}(\cdot,\cdot), g^{(m)}(\cdot,\cdot),$ and $h^{(n)}(\cdot,\cdot)$ are twice differentiable functions with respect to the first argument, $p^{(k)}ii \in [N_k]k \in [K], \quad q^{(k)}ii \in [M\ell]\ell \in [L],$ and $s^{(k)}jj \in [J\ell]_{\ell \in [L]}$ are problem data, which can either be discrete or continuous. We assume that our functions $f^{(\ell)}(\cdot,\cdot), g^{(m)}(\cdot,\cdot),$ and $h^{(n)}(\cdot,\cdot)$ can be expressed in the form of computational graphs of moderate length; that is, the resulting Lagrangian Hessian and Jacobian matrices are sparse. One can observe that the problem in (3) is expressed by a combination of the computational patterns in Section II-C.

Our implementation of the algebraic modeling interface enforces the user to specify the model equations in an Iterable data type in Julia. Julia's Iterable data type consists of the instruction and the data over which the instruction is executed. This allows maintaining the NLP problem information in the form of SIMD abstraction in (3).

Now, we discuss the key benefits of the SIMD abstraction. a) Parallel AD Implementation: The main reason for introducing a distinctive modeling abstraction in (3) is because without the abstraction, it is difficult for the AD package to detect the parallelizable structure within the model. Many of the physics-based models, such as AC OPF, have repetitive structure. One of the manifestations of it is that the mathematical statement of the model is concise, even if the model itself contains millions or even billions of variables and constraints. Specifically, it suffices to use 15 computational patterns to fully specify the model. These patterns arise from (1) generation cost, (2) reference bus voltage angle constraint, (3-6) active and reactive power flow (to and from), (7) voltage angle difference constraint, (8-9) apparent power flow limits (to and from), (10-11) power balance equations, (12-13) generators' contributions to the power balance equations, and (14-15) in/out flows contributions to the power balance equations. However, such repetitive structure is not well exploited during AD in the standard nonlinear optimization modelign tools. By preserving the repetitive structures in the model, one can facilitate the implementation of parallelized derivative

SIMDiff.jl implements the standard reverse-mode automatic differentiation. Using the multiple dispatch feature of Julia, SIMDiff.jl can generate highly efficient derivative computation code, specifically compiled for each computational pattern in the model. Furthermore, the derivative evaluation code can straightforwardly extended so that it can run over the data on acceraltor devices. In particular, the derivative computation

computations.

code is obtained as a type-stable function, which can be run on devices through array and kernel programming.

- b) Memory Efficiency: The memory footprint of storing model information can be significantly reduced with the SIMD abstraction. As opposed to storing the symbolic expressions and sparsity patterns for each constraint and objective term, which can potentially be more than millions, we only store the symbolic expression and sparsity patterns for each computational pattern. This allows drastically reducing the memory requirements. Thanks to this, our implementation has a significantly shorter model creation time and smaller memory footprint compared to the existing sparse AD tools.
- c) Efficient Symbolic Analysis: The symbolic analysis is essential in sparse automatic differentiation. This step is needed for determining the sparsity pattern of the evaluated derivatives. In sparse AD, the initial symbolic analysis of nonlinear expressions can be expensive, as the number of objective terms and constraints can be more than millions. However, often times those analyses are applied for the same computational patterns, and the time and memory spent for symbolic analysis can be significantly reduced if the SIMD-compatible computational patterns are present in the model. SIMDiff.jl exploits the SIMD abstraction of the model equations to save the computational cost spent for symbolic analysis, and this allows for efficient evaluation of derivatives without the use of the expensive symbolic analysis nor coloring procedures.

IV. CONDENSED-SPACE INTERIOR POINT METHODS WITH INEQUALITY RELAXATION STRATEGY

We present the condensed-space interior point method within the context of the general NLP formulation in (1). Our method has two key differences from standard interior point method implementations: (i) the use of inequality relaxation and (ii) the condensed treatment of the KKT system.

A. Inequality Relaxation

At the beginning of the algorithm, we apply inequality relaxation to replace the equality constraints in (1) with inequalities by introducing slack variables $s \in \mathbb{R}^m$:

$$q(x) - s = 0, \quad s^{\flat} < s < s^{\sharp}, \tag{4}$$

where $s^{\flat}, s^{\sharp} \in \mathbb{R}^m$ are chosen to be close to zero. This relaxed problem can be stated as follows:

$$\min_{\begin{bmatrix} x^{\flat} \\ s^{\flat} \end{bmatrix} \leq \begin{bmatrix} x \\ s \end{bmatrix} \leq \begin{bmatrix} x^{\sharp} \\ s^{\sharp} \end{bmatrix}} f(x)$$
 s.t. $g(x) - s = 0$. (5)

In our implementation, we set s^{\flat} , s^{\sharp} as $-\epsilon_{\text{tol}}$ and $+\epsilon_{\text{tol}}$, respectively, where $\epsilon_{\text{tol}} > 0$ is a user-specified relative tolerance of the interior point method (IPM). This type of relaxation is commonly used in practical IPM implementations; for example, in Ipopt, the solver relaxes the bounds and inequality constraints by $O(\epsilon_{\text{tol}})$ to prevent an empty interior of the feasible set (see [3, Section 3.5]). For condensed-space IPM, we cannot maintain the same level of precision due to the

increased condition number of the KKT system. We have found that setting $\epsilon_{\rm tol}$ to be $\epsilon_{\rm mach}^{1/4}\approx 10^{-4}$ ensures numerical stability while achieving satisfactory convergence. Thus, our solver sets the tolerance to 10^{-4} by default when using condensed IPM.

B. Barrier Subproblem

The barrier subproblem is considered as follows:

$$\min_{x} f(x) - \mu \mathbf{1}^{\top} \log(x - x^{\flat}) - \mu \mathbf{1}^{\top} \log(x^{\sharp} - x)$$

$$- \mu \mathbf{1}^{\top} \log(s - s^{\flat}) - \mu \mathbf{1}^{\top} \log(s^{\sharp} - s)$$
s.t. $g(x) = 0$. (6b)

Here, $\mu>0$ is the barrier parameter. The smooth log-barrier function is employed to avoid handling inequalities in a combinatorial fashion (as in active set methods). A superlinear local convergence to the first-order stationary point can be achieved by repeatedly applying Newton's step to the KKT conditions of (6) with $\mu=\mu^{(\ell)}$ and a decreasing sequence of $\mu^{(\ell)}{}_{\ell=0,1,\cdots}$. A global convergence can be achieved by employing a certain globalization strategy (either based on a merit function or filter method) [2].

C. Newton's Step Computation

The Newton step direction can be computed by considering the first-order optimality conditions for the barrier subproblem in (6):

$$\nabla_{x} f(x^{(\ell)}) - \nabla_{x} g(x^{(\ell)})^{\top} y^{(\ell)} - z_{x}^{\flat} + z_{x}^{\sharp} = 0 \qquad (7)$$

$$-z_{s}^{\flat} + z_{s}^{\sharp} = 0 \qquad g(x^{(\ell)}) = 0$$

$$Z_{x}^{\flat} (x^{(\ell)} - x^{\flat}) - \mu \mathbf{1} = 0 \qquad Z_{x}^{\sharp} (x^{\sharp} - x^{(\ell)}) - \mu \mathbf{1} = 0$$

$$Z_{s}^{\flat} (s^{(\ell)} - s^{\flat}) - \mu \mathbf{1} = 0, \qquad Z_{s}^{\sharp} (s^{\sharp} - s^{(\ell)}) - \mu \mathbf{1} = 0,$$

where $y \in \mathbb{R}^m$, $z_x^{\flat}, z_x^{\sharp} \in \mathbb{R}^n$, and $z_s^{\flat}, z_s^{\sharp} \in \mathbb{R}^m$ are Lagrange multipliers associated with the equality and bound constraints in (5). The Newton step for solving the nonlinear equation in (7) can be computed by solving the following KKT system in (8). Here, $p_x, \cdots p_{z_s^{\sharp}}$ are defined by the left-hand-sides of the equations in (7). In what follows, we shall drop the superscript $(\cdot)^{(\ell)}$ for concise notation.

Now, we observe that a significant portion of the system in (8) can be eliminated by exploiting the block structure, leading to an equivalent system stated in a smaller space. In particular, the lower-right 4×4 block is always invertible since the IPM procedure ensures that the iterates stay in the strict interior of the feasible set. This allows for eliminating the lower-right 4x4 block, resulting in:

$$\begin{bmatrix} W^{(\ell)} + \Sigma_x + \delta_w^{(\ell)} I & A^{(\ell)\top} \\ & \Sigma_s + \delta_w^{(\ell)} I & -I \\ A^{(\ell)} & -I & -\delta_c I \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta s \\ \Delta y \end{bmatrix} = \begin{bmatrix} q_x \\ q_s \\ q_y \end{bmatrix},$$
(9)

where the dependence on the evaluation point is suppressed for concise notation, and:

$$\Sigma_x := Z_x^{\flat} (X - X^{\flat})^{-1} + Z_x^{\sharp} (X^{\sharp} - X)^{-1}$$



$$\begin{split} & \Sigma_s := Z_s^{\flat} (S - S^{\flat})^{-1} + Z_s^{\sharp} (S^{\sharp} - S)^{-1} \\ & q_x := p_x + (X - X^{\flat})^{-1} p_{z_x^{\flat}} - (X^{\sharp} - X)^{-1} p_{z_x^{\sharp}} \\ & q_s := (S - S^{\flat})^{-1} p_{z_s^{\flat}} - (S^{\sharp} - S)^{-1} p_{z_s^{\sharp}} \\ & q_y := p_y. \end{split}$$

The bound dual steps can be recovered as follows:

$$\Delta z_{x}^{\flat} = \left(X - X^{\flat}\right)^{-1} \left(-Z_{x}^{\flat} \Delta x + p_{z_{x}^{\flat}}\right)$$

$$\Delta z_{x}^{\sharp} = \left(X^{\sharp} - X\right)^{-1} \left(Z_{x}^{\sharp} \Delta x + p_{z_{x}^{\sharp}}\right)$$

$$\Delta z_{s}^{\flat} = \left(S - S^{\flat}\right)^{-1} \left(-Z_{s}^{\flat} \Delta s + p_{z_{s}^{\flat}}\right)$$

$$\Delta z_{s}^{\sharp} = \left(S^{\sharp} - S\right)^{-1} \left(Z_{s}^{\sharp} \Delta s + p_{z_{s}^{\sharp}}\right) .$$

$$(10)$$

Note that the reduced system in (9) corresponds to the KKT system in (2). However, in the original version of the algorithm, we did not introduce the slack variables, so it does not have the additional structure imposed by the slack variables.

The key advantage of the inequality relaxation strategy is that it imposes additional structure in the reduced KKT system, allowing us to further reduce the dimension of the problem. In particular, the lower-right 2x2 block in (9) can be eliminated. This procedure is called *condensation*. Through this, we obtain the following system, purely written in the original primal space:

$$(W + \delta_w I + \Sigma_x + ADA^{\top}) \Delta x =$$

$$q_x + A^{\top} \left[q_s + (\delta_c \Sigma_s + (1 + \delta_c \delta_w) I)^{-1} (q_y - \delta_c q_y) \right],$$
(11)

where:

$$D := (\delta_c \Sigma_s + (1 + \delta_c \delta_w)I)^{-1} (\Sigma_s + \delta_w I).$$

The dual and slack step directions can be recovered as follows:

$$\Delta s := (\delta_c \Sigma_s + (1 + \delta_c \delta_w)I)^{-1} \left(\delta_c q_s - (q_y + A^{(\ell)} \Delta x)\right)$$

$$\Delta y := (\Sigma_s + \delta_w I)\Delta s - q_s.$$
 (12)

Therefore, the only sparse matrix that needs to be factorized is the matrix in (11), which is in $\mathbb{R}^{n \times n}$. In general NLPs, the condensation strategy can arbitrarily increase the density of the KKT system, but for AC OPF problems, the condensed KKT system is still sparse. This is because the maximum number of nonzeros per row in constraint Jacobian is bounded by the graph degree, which should be reasonably small in practice.

The reason that the condensation strategy is particularly relevant for GPUs is that the matrix in (11) is positive definite upon the application of standard inertia correction method. Typically, to guarantee that the computed step direction is a descent direction, we need a condition that $\inf(M_{\text{reduced}}) = (n+5m,0,m)$. One can observe that by applying Sylvester's law of inertia, we have:

inertia
$$(M_{\text{reduced}}) = (n + 5m, 0, m)$$

 \iff inertia $(M_{\text{cond}}) = (n, 0, 0).$

Thus, any choice of $\delta_w, \delta_c > 0$ that makes the condensed KKT system positive definite yields the KKT system with the desired inertia information. This implies that the condensed KKT matrix $M_{\rm cond}$ can be factorized with fixed pivoting (e.g., Cholesky factorization or LU factorization), which is significantly more amenable to parallel implementation than indefinite LBL^T factorization, which is commonly used in IPM on CPUs.

Typically, the system in (11) is severely ill-conditioned, and a single triangular solve may not provide a sufficiently accurate step direction. Accordingly, iterative refinement methods are employed to refine the solution by performing multiple triangular solves. Notably, iterative refinement is applied to the full KKT system (8) by using the dual step recovering procedure (10) and (12).

D. Line Search and IPM Iterations

The step size can be determined using the line search procedure. Although there are numerous alternative approaches, we follow the filter line search method implemented in the Ipopt solver [3]. The step can be implemented as follows:

$$(x, s, y) \leftarrow (x, s, y) + \alpha(\Delta x, \Delta s, \Delta y),$$

$$(z_x^{\flat}, z_x^{\sharp}, z_s^{\flat}, z_s^{\sharp}) \leftarrow (z_x^{\flat}, z_x^{\sharp}, z_s^{\flat}, z_s^{\sharp}) + \alpha_z(\Delta z_x^{\flat}, \Delta z_x^{\sharp}, \Delta z_s^{\flat}, \Delta z_s^{\sharp}).$$

$$(13)$$

The iteration in (13) is repeated until the convergence criterion is satisfied. The convergence criterion is defined as $\operatorname{residual}(x^{(\ell)}, s^{(\ell)}, y^{(\ell)}, z_x^{(\ell)}, z_x^{(\ell)}, z_x^{(\ell)}, z_s^{(\ell)}, z_s^$

Furthermore, to enhance the convergence behavior, various additional strategies are implemented, such as the second-order correction, restoration phase, and automatic scaling. For the most part, we follow the reference for the implementation of these strategies [3].

Algorithm 1 Condensed-Space Interior Point Method

Require: Primal-dual solution guesses $x, y, z^{\flat}, z^{\sharp}$, bounds $x^{\flat}, x^{\sharp}, s^{\flat}, s^{\sharp}$, callbacks $f(\cdot), g(\cdot), \nabla_x f(\cdot), \nabla_x g(\cdot), \nabla^2_{xx} \mathcal{L}(\cdot)$, and tolerance ϵ_{tol}

- 1: Relax the equality constraints by (4) and initialize the slack s and the associated dual variables $z_s^{\flat}, z_s^{\sharp}$.
- 2: while residual $(x, y, z_x^{\flat}, z_x^{\sharp}, z_s^{\flat}, z_s^{\sharp}) > \epsilon_{\text{tol}} \ \mathbf{do}$
- 3: Solve the condensed KKT system (11) to compute the primal step Δx and recover the dual steps $\Delta y, \Delta z_x^{\flat}, \Delta z_x^{\sharp}, \Delta z_s^{\flat}, \Delta z_s^{\sharp}$ by (10) and (12).
- 4: Determine the need for regularization via the inertiafree regularization procedure.
- 5: Choose a step size $\alpha > 0$ satisfying sufficient progress conditions and acceptable by filter via line search.
- 6: Compute the feasible dual step size $\alpha_z > 0$.
- 7: Update the solution by (13).
- 8: Update filter and barrier parameter μ .
- 9: end while
- 10: **return** The first-order stationary points $x^*, y^*, z^{\flat \star}, z^{\sharp \star}$

Finally, we summarize our condensed-space interior point method in Algorithm 1.

E. Notes on the Implementation

We have implemented the condensed-space IPM by adapting our code base in MadNLP.jl. In MadNLP, the IPM iteration is implemented with high levels of abstractions, while the specific handling of the data structures within the KKT systems is carried out by data-type specific kernel functions. This design allows us to run the same high-level mathematical abstractions for different data structures, such as SparseKKTSystem, DenseKKTSystem, DenseCondensedKKTSystem, etc. For the implementation of the condensed-space IPM presented in this paper, we have added a new type of KKT system called SparseCondensedKKTSystem and implemented additional kernels needed for handling the data structures specific to this KKT system type. This approach ensures that we are performing mathematically equivalent operations as in the mature, extensively tested existing code base. This also allows us to easily switch between different KKT system types, which is crucial for experimenting with various solvers and data structures, as well as for efficiently leveraging GPU acceleration when available. Furthermore, by maintaining this level of abstraction, the condensed-space IPM can be seamlessly integrated into the existing framework, making it easier to maintain and extend in the future.

V. NUMERICAL RESULTS

This section presents the numerical benchmark results, comparing our method against state-of-the-art methods on CPUs for solving standard AC OPF problems.

A. Methods

We compared four different configurations:

• MadNLP.jl + SIMDiff.jl + cuSOLVER (GPU) (Config 1)

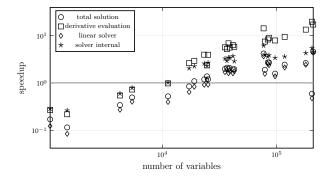


Fig. 3. Speedup achieved by using GPUs.

- MadNLP.jl + SIMDiff.jl + Ma27 (CPU) (Config 2)
- Ipopt + AMPL + Ma27 (CPU) (Config 3)
- Ipopt + JuMP.jl + Ma27 (CPU). (Config 4)

Config 1 is our main GPU configuration, and Config 2 represents our implementation running on CPU. Config 3 and Config 4 are used as benchmarks. Config 1 and Config 2 share a common code base, thanks to the multiple dispatch feature of Julia Language, but they differ in how they handle the KKT systems. In Config 1, MadNLP.il applies the condensed-space interior point method along with the inequality relaxation strategy, while in Config 2, MadNLP.jl applies factorization to the non-condensed, indefinite KKT system (as in (2)). In Config 1, we use the cuSOLVER library to solve the condensed KKT system. The initial symbolic factorization is performed using the KLU package [?]. Subsequent numerical factorization and triangular solves are performed by cuSOLVER with the fixed pivot sequence obtained from the initial factorization with KLU. Software and hardware details of each configuration are illustrated in Table I. The OPF problem is formulated using the model from the rosetta-opf project [9], and the test cases are obtained from the pglib-opf repository [10]. The external packages are called from Julia, through thin wrapper packages, such as Ipopt.jl and AmplNLWriters.jl. A tolerance of 10^{-4} is set for MadNLP.jl and Ipopt solvers, with other solver options adjusted to ensure a fair comparison across different solvers. The results can be reproduced with the script available at https://github.com/sshin23/pscc-2024-opf-gpu.

B. Results

The numerical benchmark results, including total solution time and its breakdown into linear algebra and derivative evaluation time (with the remainder considered as solver internal time), are shown in Table II. The quality of the solution (objective value and constraint violation measured by $\|\cdot\|_{\infty}$) is shown in Table III. Figure 3 visually represents the speedup brought by GPUs, comparing Config 1 and Config 2 in terms of total solution time, derivative evaluation time, and solver internal time. Key findings are as follows.

First, when comparing the solvers' performance in terms of the interior point method (IPM) iteration counts, MadNLP.jl is as efficient as the state-of-the-art solver Ipopt. The IPM

TABLE I
DETAILS OF NUMERICAL EXPERIMENT SETTINGS

	MadNLP.jl + SIMDiff.jl + cuSOLVER	MadNLP.jl + SIMDiff.jl + Ma27	Ipopt + AMPL + Ma27	Ipopt + JuMP.jl + Ma27			
	(gpu)	(cpu)	(cpu)	(cpu)			
Optimization Solver	MadNLP.jl ((dev)*	Ipopt (v3.13.3)				
Derivative Evaluations	SIMDiff.jl (dev)*	AMPL Solver Library	JuMP.jl (v1.12.0)			
Linear Solver	cuSOLVER (v11.4.5)	Ma27 (v2015.06.23)					
Hardware	NVIDIA Quadro GV100	Intel Xeon Gold 6140					

^{*}Specific commit hashes are available at https://github.com/sshin23/pscc-2024-opf-gpu

TABLE II NUMERICAL RESULTS

			MadNLP + SIMDiff + cuSOLVER			MadNLP + SIMDiff + Ma27			Ipopt + AMPL + Ma27			Ipopt + JuMP + Ma27				
Case	nvars	ncons	(gpu)			(cpu)			(cpu)			(cpu)				
			iter	deriv.†	lin.†	total [†]	iter	deriv.†	lin.†	total [†]	iter	deriv.‡	total [‡]	iter	deriv.‡	total [‡]
89_pegase	1.0k	1.6k	28	0.03	0.23	0.33	31	0.01	0.03	0.06	29	0.04	0.08	29	0.11	0.17
179_goc	1.5k	2.2k	30	0.04	0.61	0.74	43	0.01	0.05	0.09	42	0.05	0.11	42	0.15	0.24
500_goc	4.3k	6.1k	36	0.04	0.45	0.58	35	0.02	0.12	0.20	36	0.13	0.30	34	0.41	0.61
793_goc	5.4k	8.0k	33	0.03	0.36	0.49	31	0.02	0.15	0.24	31	0.19	0.37	30	0.61	0.84
1354_pegase	11.2k	16.6k	47	0.08	1.07	1.35	45	0.07	0.42	0.70	41	0.91	1.43	41	2.36	3.02
2312_goc	17.1k	25.7k	38	0.04	1.16	1.33	40	0.10	0.74	1.13	38	1.45	2.33	38	3.16	4.14
2000_goc	19.0k	29.4k	36	0.04	0.99	1.18	38	0.11	0.82	1.29	39	1.73	2.76	38	4.19	5.32
3022_goc	23.2k	35.0k	43	0.04	1.39	1.63	49	0.18	1.27	1.93	47	2.56	4.02	47	5.68	7.29
2742_goc	24.5k	38.2k	155	0.26	4.54	5.54	122	0.62	5.31	7.60	97	8.22	13.66	98	20.09	26.02
2869_pegase	25.1k	37.8k	52	0.05	1.70	1.97	52	0.21	1.56	2.35	50	3.19	4.89	50	6.07	8.00
3970_goc	35.3k	54.4k	44	0.05	1.64	1.91	45	0.26	2.77	3.75	60	5.49	10.04	43	7.20	10.92
4020_goc	36.7k	57.0k	68	0.07	2.94	3.35	59	0.36	5.66	7.01	55	5.43	11.87	55	10.72	17.54
4917_goc	37.9k	56.9k	48	0.05	1.74	2.07	57	0.34	2.79	4.07	53	5.03	7.90	53	9.84	13.07
4601_goc	38.8k	59.6k	71	0.07	2.46	2.87	66	0.41	4.37	5.92	69	6.92	12.66	68	12.82	18.74
4837_goc	41.4k	64.0k	57	0.06	2.37	2.72	56	0.39	3.79	5.24	56	6.50	10.94	56	12.70	17.61
4619_goc	42.5k	66.3k	54	0.06	2.59	2.97	46	0.32	4.54	5.78	48	5.49	11.02	46	10.04	15.48
10000_goc	76.8k	112.4k	56	0.06	2.63	3.11	77	0.89	9.54	13.00	74	14.02	24.18	74	25.13	36.46
8387_pegase	78.7k	118.7k	64	0.12	6.08	6.87	70	0.89	9.44	12.96	69	14.23	23.55	69	26.40	36.74
9591_goc	83.6k	130.6k	69	0.11	6.84	7.70	65	0.92	17.20	20.82	64	14.96	35.70	62	28.71	49.75
9241_pegase	85.6k	130.8k	60	0.10	4.35	5.15	63	0.89	10.34	13.91	61	14.09	24.33	61	25.98	37.19
10480_goc	96.8k	150.9k	70	0.13	13.19	14.26	66	1.05	18.19	22.40	64	16.93	38.04	63	33.53	56.04
13659_pegase	117.4k	170.6k	63	0.12	6.10	7.15	58	1.08	12.91	17.35	64	19.70	35.66	64	35.45	52.99
19402_goc	179.6k	281.7k	79	0.17	21.47	23.28	70	2.25	51.82	61.06	70	36.50	95.34	70	68.12	127.29
24464_goc	203.4k	313.6k	63	0.11	69.32	70.63	58	2.22	33.03	41.71	58	33.50	70.15	58	62.04	102.17
30000_goc	208.6k	307.8k	162	0.33	18.42	22.05	136	5.68	80.01	100.25	180	101.98	249.81	126	135.11	209.45

†Wall time (sec) measured by Julia. ‡CPU time (sec) reported by Ipopt.

iteration count is nearly the same as that of Ipopt for achieving the same level of accuracy in the final solution (see Table III). This suggests that running mathematically equivalent operations on GPUs can yield a similar degree of effectiveness in terms of IPM convergence.

Next, we discuss the effectiveness of parallel AD on GPUs. We observe that even on CPUs, SIMDiff.jl is substantially faster than the AD routines implemented in AMPL or JuMP.jl. This efficiency arises from SIMDiff.jl obtaining the derivative functions in the form of type-stable, compiled code. Derivative evaluation using the compiled LLVM code, specific to the model equation, generated by the Julia compiler is significantly faster than the derivative evaluations implemented in AMPL and JuMP.jl. When comparing SIMDiff.jl running on CPUs and GPUs, we observe a further speedup of up to almost 20x for large instances. This demonstrates that parallelization of AD brings significant computational gain, enabled by the SIMD abstraction of NLPs, particularly because most operations in the derivative evaluations are either Pattern 1 or Pattern 2 operations, which are highly effective on GPUs.

While the speedup achieved by linear solvers is only moderate, this has a high impact on the overall speedup, as linear solver time constitutes a significant portion of the total solution time. For large instances, approximately 4x speedup

can be achieved, though this can vary depending on the instances. For example, for case24464_goc, the GPU linear solver was slower than the CPUs. The investigation of under which circumstances cuSOLVERRF is more effective warrants further research.

Solver internal time could also be significantly accelerated through GPU utilization. We can observe that the speedup in solver internal operations is consistently greater than the speedup in linear solvers. However, due to the frequent use of Pattern 3 operations, the speedup in solver internal operations is lesser than that of derivative evaluations.

Overall, our GPU implementation exhibits significant speedup across all components: derivative evaluation, linear algebra, and solver internal computation, resulting in substantial gains in total solution time. The results indicate that GPUs become more effective for large-scale instances, particularly when the number of variables is greater than 20,000. Notably, for the largest instance, case30000_goc, our GPU implementation is 4.5 times faster than our CPU implementation and 9.5 times faster than the solver configuration with state-of-the-art tools (Ipopt, JuMP.jl, and Ma27). This demonstrates that GPUs can bring significant computational gains for large-scale AC OPF problems, enabling the solution of previously inconceivable problems due to the limitations of existing CPU-

TABLE III SOLUTION QUALITY

	MadNLP + SIMI	Diff + cuSOLVER	MadNLP + SI	MDiff + Ma27	Ipopt + AM	IPL + Ma27	Ipopt + JuMP + Ma27		
Case	(g _I	ou)	(cp	ou)	(ст	ou)	(cpu)		
	objective	constr. viol.	objective	constr. viol.	objective	constr. viol.	objective	constr. viol.	
89_pegase	1.07023029e+05	1.69977362e-03	1.07277300e+05	1.69995406e-03	1.07273132e+05	1.69762454e-02	1.07273132e+05	1.69762454e-02	
179_goc	7.54098231e+05	3.64045772e-03	7.54215279e+05	3.64095371e-03	7.54214091e+05	1.05727439e-02	7.54214091e+05	1.05727439e-02	
500_goc	4.53056588e+05	1.16442922e-03	4.54894607e+05	1.16461929e-03	4.54894301e+05	1.16449188e-03	4.54894349e+05	1.16443248e-03	
793_goc	2.59660004e+05	1.12495280e-03	2.60179408e+05	1.14373500e-03	2.60177953e+05	2.52890328e-02	2.60177960e+05	2.52825510e-02	
1354_pegase	1.25574315e+06	4.18838427e-03	1.25874608e+06	4.18894441e-03	1.25873160e+06	2.91106529e-02	1.25873160e+06	2.91106529e-02	
2312_goc	4.40492687e+05	1.95782217e-03	4.41301927e+05	1.98487972e-03	4.41301012e+05	2.86441953e-03	4.41301012e+05	2.86441953e-03	
2000_goc	9.66186544e+05	1.07957382e-03	9.73392385e+05	1.07991565e-03	9.73392524e+05	1.07970410e-03	9.73392602e+05	1.07958552e-03	
3022_goc	6.00461469e+05	1.60590210e-03	6.01341340e+05	1.92264271e-03	6.01340934e+05	7.06720510e-03	6.01340934e+05	7.06720510e-03	
2742_goc	2.70328757e+05	9.99725733e-04	2.75672815e+05	9.99997332e-04	2.75672759e+05	1.13868333e-03	2.75672759e+05	1.13868333e-03	
2869_pegase	2.45584120e+06	4.18833905e-03	2.46259584e+06	4.18882610e-03	2.46258759e+06	3.15283321e-02	2.46258759e+06	3.15283321e-02	
3970_goc	9.27998953e+05	6.41922608e-04	9.60666837e+05	6.42469892e-04	9.60667021e+05	6.42371530e-04	9.60667776e+05	6.41960999e-04	
4020_goc	8.02565861e+05	1.29969745e-03	8.21952202e+05	1.29999868e-03	8.21952543e+05	1.29986624e-03	8.21952543e+05	1.29986624e-03	
4917_goc	1.38537252e+06	1.54172485e-03	1.38769645e+06	1.70860688e-03	1.38769342e+06	1.62739725e-02	1.38769342e+06	1.62739725e-02	
4601_goc	7.92510931e+05	9.99886244e-04	8.25898288e+05	9.99978318e-04	8.25898470e+05	9.99896654e-04	8.25898481e+05	9.99894295e-04	
4837_goc	8.60071647e+05	9.92673673e-04	8.72192598e+05	9.92934504e-04	8.72192733e+05	9.92677263e-04	8.72192733e+05	9.92677263e-04	
4619_goc	4.66738422e+05	8.80364611e-04	4.76659294e+05	8.80485073e-04	4.76659432e+05	8.80367536e-04	4.76659432e+05	8.80367536e-04	
10000_goc	1.34739992e+06	5.36209615e-04	1.35370965e+06	5.40993748e-04	1.35371078e+06	6.56672045e-04	1.35371173e+06	6.56367359e-04	
8387_pegase	2.74980929e+06	9.99884691e-03	2.77083829e+06	9.99896893e-03	2.77062704e+06	5.30460965e-02	2.77062704e+06	5.30460965e-02	
9591_goc	1.02516095e+06	9.91659468e-04	1.06148769e+06	9.91997903e-04	1.06148806e+06	9.91795084e-04	1.06148807e+06	9.91788322e-04	
9241_pegase	6.21775010e+06	4.18380648e-03	6.24208171e+06	4.18787958e-03	6.24207325e+06	3.76440386e-02	6.24207325e+06	3.76440386e-02	
10480_goc	2.27696973e+06	1.09983709e-03	2.31442783e+06	1.09996886e-03	2.31442450e+06	1.67932256e-02	2.31442450e+06	1.67932256e-02	
13659_pegase	8.92385389e+06	1.99904428e-03	8.94679835e+06	1.99980680e-03	8.94680070e+06	1.54477837e-02	8.94680070e+06	1.54477837e-02	
19402_goc	1.93394723e+06	1.19983797e-03	1.97755237e+06	1.19999867e-03	1.97755235e+06	1.19986568e-03	1.97755235e+06	1.19986568e-03	
24464_goc	2.58935630e+06	7.24722104e-04	2.62932336e+06	7.24944021e-04	2.62932439e+06	7.24724162e-04	2.62932439e+06	7.24724162e-04	
30000_goc	1.11353160e+06	1.40161701e-03	1.14190983e+06	1.40292333e-03	1.14191122e+06	1.40225897e-03	1.14190714e+06	1.40184075e-03	

†Directly computed by using the callback functions. ‡Reported by Ipopt output.

based solution tools.

VI. CONCLUSIONS AND FUTURE OUTLOOK

We have presented a highly efficient nonlinear optimization framework for solving large-scale AC OPF problems. By leveraging the SIMD abstraction of NLPs and a condensedspace interior point method, we have effectively eliminated the need for serial computations, enabling the implementation of a solution framework that can run entirely on GPUs. Our method has demonstrated promising results, achieving a 4x speedup when compared to CPU implementations for large-scale optimal power flow problems. Notably, our approach outperforms one of the state-of-the-art CPU-based implementations by approximately 10 times. Therefore, our proposed computational framework, along with our packages MadNLP.il and SIMDiff.il, represents a significant advancement in scalable solution large-scale OPF problems. These findings underscore the potential of accelerated computing in large-scale optimization area, like AC OPF. However, the condensation procedure leads to an increase in the condition number of the KKT system, resulting in decreased final solution accuracy. Addressing the challenges posed by illconditioning remains an important aspect for future work. In the following paragraphs, we discuss some remaining open questions and future outlooks.

Obtaining Higher Numerical Precisions: While we have focused on the interior point method, other constrained optimization paradigms, such as penalty methods, augmented Lagrangian methods, and sequential quadratic programming, exist, and similar strategies based on condensed linear systems can be developed. It would be valuable to investigate which

one can best handle the ill-conditioning issue of the condensed KKT system and achieve the highest degree of accuracy.

Security-Constrained, Multi-Period, Distribution OPFs: Though the proposed method has demonstrated significant computational advantages for transmission AC OPF problems, efficient CPUs can still handle these problems reasonably well. We anticipate more substantial performance gains for larger-scale optimization problems, such as security-constrained and multi-period OPFs or joint optimization problems involving transmission, distribution, and gas network systems. We are interested in exploring Schur complement-based decomposition approaches, combined with the condensation-based strategy, similarly to [11], to enable even greater scalability.

Implementation of Sparse Cholesky Solver: While cu-SOLVERRF has been effective for solving the condensed KKT systems using LU factorization, Cholesky factorization holds promise for better performance due to lower computational complexity and the ability to reveal the inertia of the KKT system. We aim to explore other options for solving KKT systems, including sparse Cholesky implementations [12], [13], [7].

Portability: Our implementation is currently only tested on NVIDIA GPUs, but our GPU implementation is largely based on KernelAbstractions.jl in Julia, which should be compatible with various GPU architectures, including AMD, Intel, and Apple GPUs. By incorporating cross-architecture linear solvers, we envision achieving a portable accelerated NLP framework for different accelerator architectures.

Optimization with Data-Driven Surrogates: With the growing importance of emerging energy storage and conversion technologies like batteries and fuel cells, incorporating their physics into long-term economic performance is crucial.

Data-driven strategies are often considered due to the impracticality of first-principle modeling. Our GPU-accelerated method opens doors to the integration of data-driven surrogate models into state-of-the-art optimization frameworks. This would allow us to effectively incorporate the governing physics of these systems while benefiting from the speed and power of GPU acceleration.

REFERENCES

- [1] M. Anitescu, K. Kim, Y. Kim, A. Maldonado, F. Pacaud, V. Rao, M. Schanen, S. Shin, and A. Subramanian, "Targeting Exascale with Julia on GPUs for multiperiod optimization with scenario constraints," SIAG/OPT Views and News, 2021. [Online]. Available: http://wiki.siam.org/siag-op/images/siag-op/e/e8/ViewsAndNews-29-1.pdf
- [2] J. Nocedal and S. J. Wright, Numerical optimization. Springer, 2006.
- [3] A. Wächter and L. T. Biegler, "On the implementation of an interiorpoint filter line-search algorithm for large-scale nonlinear programming," *Mathematical programming*, vol. 106, pp. 25–57, 2006.
- [4] N. Chiang, C. G. Petra, and V. M. Zavala, "Structured nonconvex optimization of large-scale energy systems using pips-nlp," in 2014 Power Systems Computation Conference. IEEE, 2014, pp. 1–7.
- [5] J. S. Rodriguez, R. B. Parker, C. D. Laird, B. L. Nicholson, J. D. Siirola, and M. L. Bynum, "Scalable parallel nonlinear optimization with pynumero and parapint," *INFORMS Journal on Computing*, vol. 35, no. 2, pp. 509–517, 2023.
- [6] S. Shin, C. Coffrin, K. Sundar, and V. M. Zavala, "Graph-based modeling and decomposition of energy infrastructures," *IFAC-PapersOnLine*, vol. 54, no. 3, pp. 693–698, 2021.
- [7] S. Regev, N.-Y. Chiang, E. Darve, C. G. Petra, M. A. Saunders, K. Świrydowicz, and S. Peleš, "Hykkt: a hybrid direct-iterative method for solving kkt linear systems," *Optimization Methods and Software*, vol. 38, no. 2, pp. 332–355, 2023.
- [8] C. G. Petra, N. Chiang, and J. Wang, "HiOp User Guide," Center for Applied Scientific Computing, Lawrence Livermore National Laboratory, Tech. Rep. LLNL-SM-743591, 2018.
- [9] "rosetta-opf," https://github.com/lanl-ansi/rosetta-opf.
- [10] S. Babaeinejadsarookolaee, A. Birchfield, R. D. Christie, C. Coffrin, C. DeMarco, R. Diao, M. Ferris, S. Fliscounakis, S. Greene, R. Huang et al., "The power grid library for benchmarking ac optimal power flow algorithms," arXiv preprint arXiv:1908.02788, 2019.
- [11] F. Pacaud, M. Schanen, S. Shin, D. A. Maldonado, and M. Anitescu, "Parallel interior-point solver for block-structured nonlinear programs on simd/gpu architectures," arXiv preprint arXiv:2301.04869, 2023.
- [12] Y. Chen, T. A. Davis, W. W. Hager, and S. Rajamanickam, "Algorithm 887: Cholmod, supernodal sparse cholesky factorization and update/downdate," ACM Transactions on Mathematical Software (TOMS), vol. 35, no. 3, pp. 1–14, 2008.
- [13] L. Pineda, T. Fan, M. Monge, S. Venkataraman, P. Sodhi, R. T. Chen, J. Ortiz, D. DeTone, A. Wang, S. Anderson et al., "Theseus: A library for differentiable nonlinear optimization," Advances in Neural Information Processing Systems, vol. 35, pp. 3801–3818, 2022.

Government License: The submitted manuscript has been created by UChicago Argonne, LLC, Operator of Argonne National Laboratory ("Argonne"). Argonne, a U.S. Department of Energy Office of Science laboratory, is operated under Contract No. DE-AC02-06CH11357. The U.S. Government retains for itself, and others acting on its behalf, a paid-up nonexclusive, irrevocable worldwide license in said article to reproduce, prepare derivative works, distribute copies to the public, and perform publicly and display publicly, by or on behalf of the Government. The Department of Energy will provide public access to these results of federally sponsored research in accordance with the DOE Public Access Plan. http://energy.gov/downloads/doe-public-access-plan.