Exascale Grid Optimization (ExaGO) toolkit: An open-source high-performance package for solving large-scale grid optimization problems

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Abstract — This paper introduces the Exascale Grid Optimization (ExaGO) toolkit, a library for solving large-scale alternating current optimal power flow (ACOPF) problems including stochastic effects, security constraints and multi-period constraints. ExaGO can run on parallel distributed memory platforms, including massively parallel hardware accelerators such as graphical processing units (GPUs). We present the details of the ExaGO library including its architecture, formulations, modeling details, and its performance for several optimization applications.

I. INTRODUCTION

The electric power grid remains vulnerable to disruption from extreme events including wildfires, severe storms, and cyber-attacks. Variable generation resources, load volatility and system being operated closer to its limits, also present operational challenges to grid stability. To mitigate disruptions before they snowball, grid planners and operators must be able to see these events coming and understand their potential impacts on grid reliability. Planners and operators rely on optimization and real-time tools to efficiently plan and operate the grid in a secure, cost-effective manner. The foundational bedrock for this analysis has been the optimal power flow (OPF) analysis [1]–[3], which to date remains a challenging problem due to its non-convex nature.

Over the years, the complexity of the optimal power flow grew as the grid’s complexity increased and stringent reliability policies being mandated. Some examples include the incorporation of stochasticity [4], [5], N – 1 security constraints [6], [7], multi-period aspects [8], [9], and a number of modeling complexities [10], [11]. Figure 1 illustrates these three dimensions of the optimal power flow complexity.

To continue to ensure secure system operation, new tools that account for higher-level uncertainties, and are able to produce more accurate security assessment are required. Besides uncertainties, short-term decision will require additional attention, due to the more frequency ramping events caused by non-conventional generation, thus modeling that looks ahead a few steps will be desirable. Existing tools today either only address problems along a certain dimension, for e.g., security-constrained OPF only. Moreover, the scalability of such tools is limited only to a handful of “what-if condition” cases.

Fig. 1. The three uncertainty axes for the optimal power flow problem – stochasticity, security, and time. The black nodes represent optimal power flow problems along a single dimension, for e.g., stochastic optimal power flow, while the blue nodes require a combination of dimensions, for e.g., stochastic security-constrained optimal power flow. Tools addressing OPF problems along two or more dimensions at scale are needed for the future low-inertia power systems with deep penetration of renewable energy sources.

In this paper, we introduce a novel open-source tool, the Exascale Grid Optimization Toolkit (ExaGO) [12], [13], for solving Alternate Current OPF (ACOPF)-based optimization problems. The ExaGO toolkit can solve
stochastic, security-constrained, and multiperiod ACOPF problems on high-performance with CPUs and GPUs. It contains of an array of applications to solve problems along a specific dimension (for e.g. Security-constrained ACOPF) or a combination of dimensions (for e.g., stochastic security-constrained ACOPF).

ExaGO supports solving grid optimization problems expressed in general form given in (1)-(6). Here, the subscripts $s$, $c$, and $t$ represent the dimensions of stochasticity, security, and time, respectively.

$$\min \sum_{s \in S} \pi_s \sum_{c \in C} \sum_{t \in T} f(x_{s,c,t})$$

s.t.

$$g(x_{s,c,t}) = 0$$

$$h(x_{s,c,t}) \leq 0$$

$$x^- \leq x_{s,c,t} \leq x^+$$

$$-\delta_s x \leq x_{s,c,t} - x_{s,c,t,-\Delta t} \leq \delta_s x, \ t \neq 0$$

$$-\delta_c x \leq x_{s,c,0} - x_{s,0,0} \leq \delta_c x, \ c \neq 0,$$

$$-\delta_s x \leq x_{s,0,0} - x_{0,0,0} \leq \delta_s x, \ s \neq 0$$

where the subscripts $s \in S$, $c \in C$, and $t \in T$ represent the dimensions of stochasticity, contingencies, and time, respectively, and $\pi_s$ is the probability or the weight of scenario $s$. The subscript 0 denotes base-case for scenario or base-case for a contingency or the first time-period. The last three equations express the coupling between the scenarios, time, and contingencies, respectively.

ExaGO is written in C/C++ and makes heavy use of the functionality provided by the PETSc [18] library. All ExaGO applications use a nonlinear formulation based on full AC optimal power flow. The different applications available with ExaGO are listed in Table II.

| Application Name | Description                                      |
|------------------|--------------------------------------------------|
| OPFLOW           | AC optimal power flow                           |
| TCOPFLOW         | Multi-period AC optimal power flow               |
| SCOPFLOW         | Single/multi-period security-constrained AC optimal power flow |
| SOPFLOW          | Single/multi-period no/multi-contingency stochastic AC optimal power flow |
| PFFLOW           | AC power flow                                    |

The hierarchy of the applications is shown in Figure 2 to show how the applications are layered.

ExaGO is interfaced with three optimization solvers – Ipopt, HiOp, and TAO – for solving the underlying optimization problems. Figure 3 shows the solvers available for the different applications.

One unique computational feature of ExaGO is the ability to perform calculations (model evaluation and optimization solves) on the GPU. For this, it uses HiOp, RAJA [19], and Umpire [20] libraries. All the calculations are done directly on the GPU, i.e., there is minimal exchange of data between CPU and GPU during the optimization iterations. The reader is referred [21] for GPU implementation details.

In the next sections, we describe the different ExaGO applications.
III. OPFLOW: AC OPTIMAL POWER (ACOPF)

OPFLOW solves the full AC optimal power flow problem and provides various flexible features that can be toggled via run-time options. It has interfaces to different optimization solvers and includes different representations of the underlying equations (power-balance-polar and power-balance-cartesian) that can be used. By selecting the appropriate solver, OPFLOW can be executed on CPUs (in serial or parallel) or on GPUs.

In compact form, the set of equations describing ACOPF is given by (8)-(11).

\[
\begin{align*}
\min_x & \quad f(x) \\
\text{s.t.} & \quad g(x) = 0 \\
& \quad h^r \leq h(x) \leq h^+ \\
& \quad x^- \leq x \leq x^+ 
\end{align*}
\]

The full formulation of an AC optimal power flow is digressed in this paper due to space limitations. The reader is referred to [13], [15], [22] for comprehensive details on the AC optimal power flow formulation. Figure 4 briefly describes the modeling details of OPFLOW.

Fig. 4. ExaGO formulation includes standard ACOPF formulation plus feasibility (load loss, power imbalance), and advanced features (PV/PQ switching, AGC)

The layout of the ACOPF application in ExaGO is shown in Fig. 5. A clear separation of model (physics) and the solver is implemented to allow switching between different models/solvers (through run-time options). OPFLOW can be used with three different solvers: Ipopt [23], HiOp [24], [25], and TAO [18].

Different colors in Fig. 5 denote models/solvers compatible with CPU and GPU, respectively. The advantage of such a separation is that hardware-specific code for a model or a solver is isolated to it and does not spill over other portions of the code base and can be easily replaced.

IV. TCOPFLOW: MULTI-PERIOD OPF

TCOPFLOW solves a full AC multi-period optimal power flow problem with the objective of minimizing the total cost over the given time horizon while adhering to constraints for each period and between consecutive time-periods (ramping constraints).

The multi-period optimal power flow problem is a series of optimal power flow problems coupled via temporal constraints. The generator real power deviation \((p_{gt} - p_{gt-\Delta t})\) constrained within the ramping limits form the temporal constraints.

An illustration of the temporal constraints is shown in Fig. 6 with four time steps. Each time-step \(t\) is coupled with its preceding time \(t - \Delta t\), where \(\Delta t\) is the time-step where the objective is to find a least cost dispatch for the given time horizon.

\[
\begin{align*}
\min & \quad \sum_{t \in T} f(x_t) \\
\text{s.t.} & \quad g(x_t) = 0 \\
& \quad h(x_t) \leq 0 \\
& \quad x^- \leq x_t \leq x^+ \\
& \quad -\delta_t x_t \leq x_t - x_{t-\Delta t} \leq \delta_t x_t, \quad t \neq 0
\end{align*}
\]

TCOPFLOW currently supports solving the multi-period OPF problem using Ipopt on single processor...
only. Figure 7 shows the results from TCOPFLOW for a 30-min. horizon with 5 minute intervals for the ACTIVSg200 [26] bus system.

![Figure 7](image)

Fig. 7. Generation dispatch for ACTIVSg200 [26] bus system from TCOPFLOW for a 30-min horizon with 5-minute intervals.

Load and/or wind generation profiles can be set for the multiperiod problem with TCOPFLOW. The output of the base-case and the contingency subproblems is saved to MATPOWER format files (one file per subproblem).

V. SCOPFLOW: SINGLE/MULTI-PERIOD SECURITY-CONSTRAINED ACOPF

SCOPFLOW solves a single/multi-period contingency-constrained optimal power flow problem. The problem is set up as a two-stage optimization problem where the first-stage (base-case \(c_0\)) represents the normal operation of the grid and the second-stage comprises \(c \in C\) contingency cases. Each contingency case can be single or multi-period. SCOPFLOW operates in two modes: (a) preventive - only reference generators pick up the deficit/excess power for the contingency, or (b) corrective - the generators are allowed to ramp up/down constrained by their ramping limits. In the next subsections, we described the single-period and multi-period formulations for SCOPFLOW.

A. Single-period

The contingency-constrained optimal power flow (popularly termed as security-constrained optimal power flow (SCOPF) in power system parlance) attempts to find a least cost dispatch for the base case (or no contingency) while ensuring that if any of contingencies do occur then the system will be secure. This is illustrated in Fig. 8 for a SCOPF with a base-case \(c_0\) and three contingencies.

![Figure 8](image)

Fig. 8. Contingency constrained optimal power flow example with three contingencies. \(c_0\) represents the base case (or no contingency case). \(c_1, c_2, c_3\) are the three contingency cases. Each of the contingency states is coupled with the base-case through ramping constraints (denoted by red lines).

In set \(C\), i.e., \(C \equiv C \cup c_0\). Equation (21) represents the coupling between the base-case and each of the contingency states \(c_i\). Equation (21) is the most typical form of coupling that limits the deviation of the contingency variables \(x_c\) from the base \(x_0\) to within \(\delta_c x\). An example of this constraint could be the allowed real power output deviation for the generators constrained by their ramp limit.

\[
\min \sum_{c \in C} f(x_c) \quad (17)
\]

\[
\text{s.t.} \quad g(x_c) = 0, \quad (18)
\]

\[
h(x_c) \leq 0, \quad (19)
\]

\[
x^- \leq x_c \leq x^+, \quad (20)
\]

\[
-\delta_c x \leq x_c - x_0 \leq \delta_c x, \; c \neq 0 \quad (21)
\]

where, \(C\) represents the set of contingencies, including the base-case denoted by subscript 0. The list of contingencies is provided through a PTI or native format file. Each contingency can be single outage (e.g. single generator outage) or multiple (e.g. simultaneous generator and a line outage).

Three different solvers are available to solve single-period SCOPFLOW:

- With the Ipopt solver, SCOPFLOW constructs a large monolithic problem consisting of the base case and the contingencies. This solver is only supported in serial.
- The HiOp solver uses a primal decomposition approach to parallelize SCACOPF analysis where each contingency problem (and base case) are solved independently. HiOp uses a primal decomposition approach with second order corrections [27] to solve the SCOPFLOW problem. This solver is supported in serial and parallel, and can also use GPUs for solving the contingency subproblems. Figure 9 shows strong scaling of SCOPFLOW with HiOP primal decomposition algorithm on the AC-
TIVSg200 [26] test system with 100 contingencies.

- The EMPAR solver is an *embarrassingly parallel* version of SCOPFLOW that solves the base case and contingency subproblems independently in parallel. In other words, it relaxes the coupling constraint between the base-case and contingency subproblems and solves them separately. Figure 10 shows the scalability of the embarrassingly parallel solver for a large-scale optimization run.

**B. Multiperiod**

In the multi-period version of SCOPFLOW, each contingency comprised of multiple time-periods. The multiple periods have variables and constraints as described in section IV, i.e., each multiperiod problem uses TCOPFLOW application internally. An example of multi-contingency multi-period optimal power flow is illustrated in Fig. 11 with two contingencies \( c_0 \) and \( c_1 \). Here, \( c_0 \) is the case with no contingencies, i.e., the base-case. In this example, each contingency is multi-period with four time-periods. Each time-step is coupled with its adjacent one through ramping constraints. Currently, we assume the contingency is incident at the first time-step, i.e. at \( t_0 \). This results in the coupling between the contingency cases \( c \in C \) and the base-case \( c_0 \) only at time-step \( t_0 \) as shown in Fig. 11.

The overall objective of this contingency-constrained multi-period optimal power flow is to find a secure dispatch for base-case \( c_0 \) while adhering to contingency and temporal constraints. The general formulation of this problem is given in Eqs. (22) – (28).

\[
\min \sum_{c \in C} \sum_{t \in T} f(x_{c,t}) \tag{22}
\]
\[
\text{s.t.}
\]
\[
g(x_{c,t}) = 0 \tag{23}
\]
\[
h(x_{c,t}) \leq 0 \tag{24}
\]
\[
x^- \leq x_{c,t} \leq x^+ \tag{25}
\]
\[
-\delta_c x \leq x_{c,t} - x_{c,t-\Delta t} \leq \delta_c x, \ t \neq 0 \tag{26}
\]
\[
-\delta_c x \leq x_{c,0} - x_{0,0} \leq \delta_c x, \ c \neq 0 \tag{27}
\]
\[
\tag{28}
\]

here, \( C \) and \( T \) are the sets for contingencies (including the base-case) and time-steps, respectively.

The objective of the multi-period SCOPFLOW formulation is to reduce the total cost for the given horizon over the set of contingencies. Equation (28) represents the coupling between the base case \( c_0 \) and each contingency \( c_i \) at time-step \( t_0 \). We use a simple box constraint \( \delta_c x \) to restrict the deviation of decision variables \( x_{c,0} \) from the base-case \( x_{0,0} \). The bound \( \delta_c x \) could represent here, for example, the allowable reserve for
each generator. All the modeling details of TCOPFLOW IV can be used for this multi-period setup. The multi-period SCOPFLOW currently supports solution using Ipopt only. It can also do an embarrassingly parallel solution where the contingency coupling constraints are relaxed and each multi-period problem is distributed and solved independently on a rank.

VI. SOPFLOW: Single/Multiperiod No/Multi-contingency Stochastic ACOPF

SOPFLOW solves a stochastic optimal power flow problem where the stochasticity is described through scenarios of wind and/or load forecast deviations. The problem is set up as a two-stage optimization problem where the first-stage (base-case) represents the normal operation of the grid (or the most likely forecast) and the second-stage comprises $N_s$ scenarios of forecast deviation. Each scenario can have multiple contingencies and each contingency can be multi-period. Like SCOPFLOW, SOPFLOW also operates in either a preventive or corrective mode of generation redispatch.

In the next subsections, we describe the different variations of SOPFLOW.

A. Single period, no contingencies

This problem has a structure as illustrated in Fig. 12.

![Fig. 12. Stochastic optimal power flow example with three four. $s_0$ represents the base case (or the scenario with the highest probability). $s_1$, $s_2$, $s_3$ are the other three scenario forecasts. Each of the scenarios is coupled with the base-case scenario through ramping constraints (denoted by red lines)](image)

The formulation for the single period stochastic optimal power flow is given in 29–33. This formulation is similar to single-period SCOPFLOW. The difference is SOPFLOW objective is weighted by $\pi_s$ for each scenario.

$$\min \sum_{s \in S} \pi_s f(x_s)$$

s.t.

$$g(x_s) = 0,$$  

$$h(x_s) \leq 0,$$  

$$x^- \leq x_s \leq x^+,$$  

$$-\delta_x x \leq x_s - x_0 \leq \delta_x x, \ s \neq 0$$

here, $S$ is the set of scenarios with the base-scenario denoted by subscript 0. While there is no real notion of a “base” scenario, our current implementation assumes it as the scenario with the most weight or probability. The coupling constraints between the base-case and scenario subproblem are ramping constraints for the generators.

The single period, no contingency SOPFLOW can be solved on a single processor (serial) with Ipopt, in parallel using HiOp primal decomposition approach, or in an embarrassingly parallel way with the EMPAR solver.

B. Single period, multiple contingencies

The aim of the single period, contingency-constrained stochastic OPF is to optimize the grid dispatch to ensure the grid is secure for all the wind forecast deviations and for all the contingencies considered therein. There are two variations of this problem implemented in ExaGO differing in how the contingency-scenario pairs are set up.

1) Full stochastic contingency-constrained structure: (34)-(39) describes the formulation for the full stochastic contingency-constrained OPF formulation and its structure is illustrated in Figure 13 with a two scenarios–two contingency example.

![Fig. 13. Full stochastic contingency-constrained optimal power flow structure](image)
\[
\begin{align*}
\min \sum_{s \in S} \pi_s \sum_{c \in C} f(x_{s,c}) & \quad \text{(34)} \\
\text{s.t.} & \\
g(x_{s,c}) = 0, & \quad \text{(35)} \\
h(x_{s,c}) \leq 0, & \quad \text{(36)} \\
x^- \leq x_{s,c} \leq x^+, & \quad \text{(37)} \\
-\delta_s x \leq x_{s,0} - x_{0,0} \leq \delta_s x, \ s \neq 0 & \quad \text{(38)} \\
-\delta_c x \leq x_{s,c} - x_{s,0} \leq \delta_c x, \ c \neq 0 & \quad \text{(39)}
\end{align*}
\]

### C. Flattened stochastic contingency-constrained structure

This variation is a relaxation of the full structure obtained by flattening the contingency-scenario pairs to reduce the problem to a two-stage optimization problem. The formulation is given in (34)-(39) and its structure is illustrated in Figure 14.

\[
\begin{align*}
\min \sum_{s \in S} \pi_s \sum_{c \in C} f(x_{s,c}) & \quad \text{(40)} \\
\text{s.t.} & \\
g(x_{s,c}) = 0, & \quad \text{(41)} \\
h(x_{s,c}) \leq 0, & \quad \text{(42)} \\
x^- \leq x_{s,c} \leq x^+, & \quad \text{(43)} \\
-\delta_s x \leq x_{s,0} - x_{0,0} \leq \delta_s x, \ s \neq 0 & \quad \text{(44)} \\
-\delta_c x \leq x_{s,c} - x_{s,0} \leq \delta_c x, \ c \neq 0 & \quad \text{(45)}
\end{align*}
\]

### D. Multiperiod, multi-contingency

This is the most detailed formulation involving stochasticity, security constraints, and time, i.e. all the three dimensions of uncertainty. The full formulation for the stochastic security-constrained multi-period optimal power flow is given in (46) – (52). In this formulation, the objective is to reduce the expected cost, where \( f(x_{s,c,t}) \) is the cost for scenario \( s \) with contingency \( c \) at time \( t \). \( \pi_s \) is the probability of scenario \( s \).

\[
\begin{align*}
\min \sum_{s \in S} \pi_s \sum_{c \in C} \sum_{t \in T} f(x_{s,c,t}) & \quad \text{(46)} \\
\text{s.t.} & \\
g(x_{s,c,t}) = 0 & \quad \text{(47)} \\
h(x_{s,c,t}) \leq 0 & \quad \text{(48)} \\
x^- \leq x_{s,c,t} \leq x^+ & \quad \text{(49)} \\
-\delta_t x \leq x_{s,c,t} - x_{s,c,0-\Delta t} \leq \delta_t x, \ t \neq 0 & \quad \text{(50)} \\
-\delta_c x \leq x_{s,c,0} - x_{s,c,0} \leq \delta_c x, \ c \neq 0 & \quad \text{(51)} \\
-\delta_s x \leq x_{s,0,0} - x_{s,0,0} \leq \delta_s x, \ s \neq 0 & \quad \text{(52)}
\end{align*}
\]

Fig. 15. Scalability of SOPFLOW using primal decomposition approach. The HIOP solver was used for solving SOPFLOW on the ACTIVSg200 system with 5 wind scenarios and 100 contingencies.
An illustration of SOPFLOW is shown in Fig. 16 for a case with two scenarios $s_0$ and $s_1$. Each scenario has two contingencies $c_0$, $c_1$, and each contingency has four time-periods.

![Illustration of SOPFLOW](image)

Fig. 16. Stochastic multi-period contingency constrained example with two scenarios $s_0$ and $s_1$. Each scenario has two contingencies $c_0$ and $c_1$ and each contingency consists of four time-periods $t_0, t_1, t_2, t_3$. State $s_0, c_0, t_0$ represents the base case (no contingency) case for the two scenarios. We assume that any contingency is incident at the first time-step, i.e., at $t_0$. Thus, the contingency states $c_1, t_0$ is coupled with the no-contingency state $c_0, t_0$ at time $t_0$ for both the scenarios. The red line denotes the coupling between the contingency and the no-contingency states. The blue line denotes the coupling between the scenarios.

SOPFLOW currently only supports Ipopt solver to solve the stochastic security-constrained multi-period optimal power flow problem.

VII. CONCLUSIONS AND FUTURE WORK

Dealing with increased uncertainties will be important to address reliability issues in a deep decarbonized grid with low-inertia and extensive penetration off renewable energy sources. The ExaGO toolkit aims to solve large-scale stochastic, security-constrained, multi-period ACOPF problems on high-performance computers. It has high-fidelity models with scalable numerical algorithms. Moreover, it has a well-designed API through which new models and solvers can be interfaced. ExaGO has been validated against PowerWorld [29] on several test networks and we are continually validating it on more networks and applications. It is in active development and several new features are to be added to the library including new modeling capabilities (storage, flexible load), improving robustness for large-scale optimization problems, and high-performance implementation of multi-period, multi-contingency stochastic ACOPF, and expanding its solver capabilities.

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