The GridPACK™ Toolkit for Developing Power Grid Simulations on High Performance Computing Platforms

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ABSTRACT
This paper describes the GridPACK™ framework, which is designed to help power grid engineers develop modeling software capable of running on high performance computers. The framework contains modules for setting up distributed power grid networks, assigning buses and branches with arbitrary behaviors to the network, creating distributed matrices and vectors, using parallel linear and non-linear solvers to solve algebraic equations, and mapping functionality to create matrices and vectors based on properties of the network. In addition, the framework contains additional functionality to support IO and to manage errors. The goal of GridPACK™ is to provide developers with a comprehensive set of modules that can substantially reduce the complexity of writing software for parallel computers while still providing efficient and scalable software solutions.

Keywords
Electric Power Grid, High Performance Computing, Software Frameworks

1. INTRODUCTION
The electric power grid has been characterized as being the largest machine in the world, but in spite of this it is still being modeled primarily on workstations running serial programs. Much smaller systems (e.g. the internal combustion engine[4]), on the other hand, are being modeled in ways that can fully exhaust the resources of the largest available computing systems. Power grid engineers have spent enormous effort and ingenuity reducing simulations of the grid to manageable sizes, but these reductions have resulted in approximations and loss of detail which may be hiding or obscuring important features and behaviors of the power network. Furthermore, as the power grid becomes more complicated, due to more varied and unpredictable energy sources such as wind and solar energy and the influx of more information from data sources such as smart meters, the task of modeling even small networks becomes more challenging. The power grid is clearly an appealing target for high performance computing (HPC) but there are few tools available to assist power grid engineers interested in writing code to run on HPC platforms.

This paper will describe the GridPACK™ framework for developing parallel power grid simulations that run on HPC platforms with high levels of performance and scalability. Frameworks have appeared in other contexts and been used to reduce the programming burden on domain scientists by making complex but commonly used motifs available through libraries or other mechanisms. Both the Community Climate System Model[6] and Weather Research and Forecasting Model[13] are framework-based approaches to developing climate and weather models. The Cactus framework is designed to support grid-based applications and is widely used in the numerical general relativity community[8]. The Common Component Architecture[2] is a framework designed to support modularization of codes and has been used successfully in some groundwater applications[14]. Other examples of frameworks or modular approaches to code development can be found, particularly among large software projects with a broad developer base.

The GridPACK™ toolkit is designed to allow power system engineers to focus on developing working applications from their models without getting bogged down in the details of decomposing the computation across multiple processors, managing data transfers between processors, working out index transformations between power grid networks and the matrices generated by different power applications, and managing input and output. GridPACK™ encapsulates as much of the book-keeping required to set up HPC applications as possible in high-level programming abstractions that allow developers to concentrate on the physics and mathematics of their problems. The following will summarize the overall design of the GridPACK™ framework and then describe the major modules that have been developed so far.
2. POWER GRID REQUIREMENTS

The initial focus of the GridPACK™ design analysis was to target four power grid applications and to identify common features that span multiple applications. This analysis included a breakdown of the application into phases and identification within each phase of the functionality required to complete them. The four applications originally targeted within this project were power flow simulations[9], contingency analysis[5], state estimation[1] and dynamic simulation[11]. This analysis identified three major categories of functionality that required support from the framework and a number of smaller categories that were extremely useful. The categories are:

- Distributed graphs representing the network topology of the power grid and flexibility in specifying the behavior of objects located on the network. The power grid network is represented as a graph with edges referred to as branches and nodes referred to as buses.
- Distributed matrices and vectors and parallel solvers and preconditioners. The solution algorithms for power grid problems are usually expressed in terms of linear or non-linear algebraic equations.
- Mapping objects located on the network to distributed matrices and vectors. For example, the diagonal elements of the admittance matrix are associated with buses and the off-diagonal elements are associated with branches. The mapping between the network and matrix elements can be automated to a considerable extent.

These three areas encompass two major classes of data objects, distributed networks and distributed matrices and vectors. One of the goals of GridPACK™ was to create support for these data objects and transformations between the two.

The network topology is the starting point for any power grid analysis. The topology defines the initial network model and is the connection point between the physical problem definition in terms of buses and branches and the solution method, which is usually expressed in terms of matrices and vectors. Because the network is expected to be a large data object, it is undesirable to replicate it across processors. Instead, the network is divided across processors to both minimize the memory utilization on each process and to minimize communication volume between processors. The GridPACK™ framework needs to support the distribution of the network along with the exchange of data that is required between processors. Data exchanges are required because parts of the network located on one processor need to access the buses and branches they are attached to that reside on other processors. This is particularly true for problems that rely on an iterative loop for their solution where network exchanges need to occur at each iteration.

The network also serves as a container for the objects that define the behavior of buses and branches in the actual power grid model. These objects represent the physical system being modeled as well as the analyses that are being performed on it. All the things that might be present on a bus or branch, such as generators, loads, grounds, transformers, sensors, etc. need to be contained within the bus and branch objects. Bus and branch behaviors frequently depend on the objects immediately attached to them so that buses depend on the branches that are attached to them (and possibly on the buses attached to them via a branch) and branches depend on the buses attached at either end of the branch. Providing easy access to these attached objects is another function of the network module.

Basic algebraic objects, such as matrices and vectors, are a core part of the solution algorithms required by power grid analyses. These also tend to be large data objects that must be distributed across processors. Furthermore, the solution algorithms built around these data objects are generally the most time consuming part of program execution, so it is necessary to ensure that the solutions are fully parallel as well. Most solution algorithms are dominated by sparse matrices but a few, such as Kalman filter analyses[12], require dense matrices. Vectors are typically dense. There exists a rich set of libraries for constructing distributed matrices and vectors and these also contain preconditioner and solver capabilities. GridPACK™ leverages this work heavily by creating wrappers around these libraries to create matrices and vectors that can be used in solution algorithms. Wrapping these libraries instead of using them directly has the advantage that creating these algebraic objects can be simplified somewhat for power grid applications but more importantly, it allows developers to investigate new solver and algebraic libraries seamlessly without disrupting other parts of the code. The current GridPACK™ implementation is built on top of the PETSc[3] libraries but other possibilities include Hypre[7] and Trilinos[10]. All these libraries support distributed matrices and vectors, basic algebraic operations such as matrix-vector multiply, inner products, etc. and a variety of solution methods for linear and non-linear equations.

Finally, there is a need to support generation of matrices from objects in the network and the ability to push data from solution vectors back down into network objects. This is one of the most complicated and error-prone parts of writing code, especially for parallel platforms. Much of the work involved in setting up matrices can be eliminated by having users implement a few functions that provide individual matrix elements contributed by each bus or branch. The mapping function can then assemble these elements into a complete matrix for the entire system. The fact that developers can focus on writing code for individual matrix elements reduces the amount of programming required and fits in more intuitively with the physical models. The complicated index calculations required to evaluate global offsets that are needed to set up a distributed matrix can be left to the framework.

3. GRIDPACK™

This section will describe the core components identified so far and the functionality they will support. It will start off with two components that directly support the major underlying data objects, the power grid network and its associated data fields and matrices and vectors. Additional components are then built on top of these (or at least in conjunction with them). These include a partitioner to divide the network among processors, network components that describe the physics of the different network models and/or analyses.
formats. GridPACK™ allows developers to import and export data using standard formats. GridPACK™ is currently implemented as a C++ library and is designed to be run on Linux platforms (the standard OS for most HPC architectures). The library currently has no interface for Windows-based computers, but we believe it will be possible to develop such a capability in the future if there is a demand for it.

Many of these components rely heavily on external libraries to minimize framework development time and to capitalize on the considerable investment in time and expertise invested in them. By wrapping these libraries in interfaces geared towards power grid applications they can be made easier to use by power grid engineers. The interfaces also make it possible to swap out libraries in the future for new or improved implementations of specific functionality without requiring application developers to rewrite their codes. This can significantly reduce the cost of introducing new technology into the framework and allows application specific or vendor-proprietary algorithms to be incorporated easily into the framework. Core framework components are described below.

3.1 Network Module
The network module is a templated class that can be created using any type of model for the buses and branches. The network class has four major functions

- The network is a container for the network topology. The connectivity of the network is maintained by the network object and can be made available through requests to the network. The network also maintains the “ghost” status of locally held buses and branches and determines whether a bus or branch is owned by a particular processor or represents a ghost image of a bus or branch owned by a neighboring processor.

- The network topology can then be decorated with bus and branch objects that reflect the properties of the particular physical system under investigation. These bus and branch objects are written by the application developer and model the physical system and the analyses that need to be performed on it. Different applications will use different bus and branch implementations.

- The network module is responsible for implementing update operations that can be used to fill in the value of ghost cell fields with current data from other processors. The updates of ghost buses and ghost branches have been split into separate operations to give users flexibility in optimizing performance by minimizing the amount of data that needs to be communicated in the code.

- The partitioner is responsible for distributing the network among processors in such a way that each processor has roughly equal numbers of buses and branches and so that buses and branches on the same processor are mostly connected and connections to buses and branches on other processors are minimized. This layout will optimize the communication efficiency between processors by minimizing the number of processors that need to communicate with each other and reducing the amount of data that must be exchanged between processors.

The combination of the functionality described above will make it possible to build arbitrary network-based data structures and to use them in parallel applications. The complexity of working with the distributed network is comparable to the complexity of working with a serial application.

3.2 Math Module
The math module is used to create distributed matrices and vectors and also implements linear and non-linear solvers and their preconditioners. The math module is designed to be a thin wrapper on top of existing parallel math libraries. It is currently implemented using PETSc but could be implemented using other libraries. Other implementations would not require changes to other parts of the GridPACK™ framework or to existing applications.

The math module consists of routines for generating distributed matrices and vectors as well as routines for using them in linear and non-linear solvers. Creating a matrix or vector generally consists of 1) creating the matrix or vector object 2) adding elements to the objects using global indices and 3) assembling the object into a state where it can be used in solvers. This operation allows the libraries to set up internal data structures that handle distribution of the matrix or vector and control communication in parallel algebraic operations. Once matrices and vectors have been created, they can be treated as opaque objects and manipulated using a high level API that would be comparable to writing Matlab code.

In addition to allowing user to create algebraic objects, the module supports basic algebraic operations such as matrix-vector multiplies, scaling of matrices and vectors, evaluation of norms, etc. The library can also be used to create linear and non-linear solvers. Linear solvers are can be used directly on matrices and vectors but non-linear solvers require the creation of specific functions that are used inside the non-linear solver to update the solutions at each solver cycle.

3.3 Network Components
Network component is a generic term for objects associated with buses and branches. These objects determine the behavior of the system and the type of analyses being done. Branch components can represent physical objects such as transmission lines and transformers while bus components can model loads, generators, or something else. Both kinds of components could represent measurements (e.g. for a state estimation analysis).

Network components cover a broad range of behaviors and there is little that can be said about them outside the context of a specific problem. Each component inherits from a
The Y-matrix is expressed as a complex matrix, then the blocks are of size 1×1. The location of these blocks in the matrix is determined by the location of the corresponding buses and branches in the network, but the indexing calculations required to determine this location can be made completely transparent to the user via the mapper module.

Because the matrix-vector interface focuses on small blocks, it is relatively easy for power grid engineers to write the corresponding methods. The full matrices and vectors can then be generated from the network using simple calls to the mapper interface. For example, the equation for contributions from transmission elements on branches to the off-diagonal elements of the Y-matrix is:

$$Y_{branch_{mn}} = \sum_k -\frac{1}{r_{mnk} + jx_{mnk}}$$

where \( r_{mnk} \) is the resistance for the \( k \)th transmission element going from bus \( m \) to bus \( n \), \( x_{mnk} \) is the reactance of the \( k \)th transmission element from bus \( m \) to bus \( n \) and \( j = \sqrt{-1} \). The sum is over the transmission elements connecting \( m \) and \( n \). Information on all transmission elements between \( m \) and \( n \) is already located on the \( mn \) branch so this calculation is purely local.

The contributions from buses and branches to the diagonal elements of the Y-matrix can be written as

$$Y_{bus_{mm}} = S_{bus_{mm}} - \sum_{n \neq m} Y_{branch_{mn}}$$

Equation (2) is evaluated by looping over branches that are connected to bus \( m \). The quantities \( S_{bus_{mm}} \) represent other contributions to \( Y_{bus_{mm}} \) from sources other than transmission lines. The evaluation of these contributions is straightforward since the BaseBusComponent and BaseBranchComponent classes already contain methods for getting a list of all branches attached to a bus or the buses attached to either end of a branch. The bus contribution calculation consists of 1) getting a list of the branch objects connected to the bus 2) looping over these objects and obtaining the value of \( Y_{branch_{mn}} \) from them and 3) accumulating these into \( Y_{bus_{mm}} \).

The matrix-vector interface contains a number of functions that are important for building matrices. These are divided into two sets. The first reports back on the size of the block that the bus or branch contributes to the matrix, the second provides the actual values in the block. To construct the Y-matrix as a real, \( 2N \times 2N \) matrix, where \( N \) is the number of buses in the network, the size method for the diagonal elements (buses) and off-diagonal elements (branches) returns the value 2 for both dimensions of the block and the values method returns the block

$$\begin{bmatrix} a & -b \\ b & a \end{bmatrix}$$

where \( a \) and \( b \) the real and imaginary parts of either \( Y_{bus_{mm}} \) (for buses) or \( Y_{branch_{mn}} \) (for branches). If the appropriate functions in the matrix-vector interface have been implemented in the bus and branch components, then matrices and vectors will automatically be built by the mapper component.

The class structure for the network components is shown in Figure 1. Of these base classes, the MatVect Interface is the most important. It answers the question what block of data is contributed by a bus or branch to a matrix and what the dimensions of the block are. For example, for powerflow simulations it is necessary to construct an entity known as the Y-matrix. If a real-valued formulation, the grid components on branches contribute a 2×2 block to the diagonal of the Y-matrix. Similarly, the grid components on branches contribute a 2×2 block to the off-diagonal elements. If the

![Figure 1: An inheritance diagram for the network component classes. The base class for all network components is the MatVect Interface which defines functions that can be overwritten by network components to produce matrices and vectors used in computations. The BaseComponent, BaseBusComponent and BaseBranchComponent classes define generic functions that are useful in calculations. These include routines for obtaining neighboring buses or branches.](image-url)
3.4 Mapper Module

The mapper module contains a number of objects that can be used to generate matrices and vectors from network components. The mappers scan the matrix-vector interface functions in the network components and use the information provided by them to create the corresponding matrices. The size information and the location of the component in the network allows the mapper to calculate the location of the element(s) in the matrix and the remaining functions provide the actual matrix values. The matrix mapper is illustrated in Figure 2 for a small network. Figure 2(a) shows a hypothetical network for which some buses and branches do not contribute to the matrix as seen if Figure 2(b). In addition, not all buses and branches contribute the same size blocks. The mapping of the individual contributions from the network in Figure 2(b) to initial matrix locations based on network location is shown in Figure 2(c). This is followed by the elimination of gaps in the matrix due to rows and columns with no values in Figure 2(d).

The vector mappers are similar to the matrix mappers and are used to construct a vector from functions that are defined on the buses. The vector mapper can also be used to push values from a vector back onto the buses. This is important in iterative or non-linear solver where the matrices need to be updated based on the solutions of the previous iteration. The solutions are first pushed back down on to the buses in the network. The network then exchanges data between processors and based on the new values in the buses, new matrices and vectors are produced for the next iteration.

The matrix and vector mappers can eliminate an enormous amount of complex programming required to set up distributed matrices and indices. In combination with the network and math modules, it also allows developers to write code that is fully distributed at all stages of the calculation. This will minimize memory utilization as well as communication and redundant computation. All these are important in developing computationally efficient and scalable code.

3.5 Other Framework Components

The network, math, and mapper modules are the most important parts of the GridPACK™ framework, but other modules have been added that may simplify many aspects of code development. A brief description of these components follows.

3.5.1 Factories

The factory component is an application specific component that is subclassed from a factory base class. Factories manage interactions between the network and the network components. For example, it is desirable that each network component has methods that allow it to return a list of the network components to which it is directly attached. However, topology information is stored in the network. The base factory class has a method that works in conjunction with methods in the base component class to set up internal data structures so that this capability is available in each network component. Other functionality of this type could be added based on the needs of individual applications. A common type of function is something that runs over all bus and branch components in the network and triggers a method in each bus and/or branch.

Figure 2: A schematic diagram of the matrix map function. The bus numbers in (a) and (b) map to approximate column locations in (c). (a) a small network (b) matrix blocks associated with branches and buses. Note that not all blocks are the same size and not all buses and branches contribute (c) initial construction of matrix based on network indices (d) final matrix after eliminating gaps.
3.5.2 Import Module
The import module is designed to read an external network file and set up the network topology. It also associates all parameters assigned to each bus and each branch to the bus or branch as a collection of key-value pairs. These pairs are then used to instantiate the corresponding network components. The import module does not partition the network, it is only responsible for reading in the network and distributing the different network elements in a way that guarantees that not too much data ends up on any one processor. Currently, GridPACK supports the PSS/E PTI version 23 format but import modules supporting other data formats could be written and easily substituted for the PTI format. We are currently investigating other formats for inclusion into GridPACK™.

3.5.3 Serial IO Module
The serial IO module can be used to write data to standard output. It is used primarily for exporting parameters associated with buses and branches in a list format to either the screen or to a file. The user is required to write a function that formats the output from a bus or branch into a single character string and the serial IO module makes sure that the data is moved to the head processor and written out in a consistent order.

3.5.4 Configuration Module
The configuration module is designed to provide a central mechanism for directing module specific information to each of the components making up a given application. This information is typically associated with a standard input file and contains information such as the convergence threshold or the maximum numbers of iterations that could be used in the solution. The configuration module reads the external file and broadcasts the information to all processors. It can subsequently be queried anywhere in the program to extract parameters that might be needed by a particular module. The configure module supports input files using an XML syntax. This choice was made to enable interoperability between applications written using GridPACK™ and other workflow and data management tools being developed for power grid modeling.

4. APPLICATION EXAMPLE
A brief sketch of an actual powerflow example is shown in Figure 3. Namespaces and other details that would be present in an actual application have been suppressed for brevity and clarity. Line 1 defines an application-specific network type based on the component classes PFBus and PFBranch. Most of the work in actually creating an application is focused on writing these classes. The PFNetwork object is instantiated using a default communicator and then used to create an import module object in line 6. This object imports an network configuration file ("network.raw" in this example) and then partitions the resulting network among the available processors in line 8. The code then creates an application factory and uses it to instantiate the network components in line 11. It also sets up various indices and buffers used by the mapper routines and ghost exchanges in lines 12 and 13. The network exchanges between buses is initialized in line 15. Each of the buses and branches then performs a calculation to evaluate the components of the network.

```cpp
typedef BaseNetwork<PFBus,PFBranch> PFNetwork;
Communicator world;
shared_ptr<PFNetwork> network(new PFNetwork(world));
PTI23_parser<PFNetwork> parser(network);
parser.parse("network.raw");
network->partition();
PPFactory factory(network);
factory.load();
factory.setComponents();
factory.setExchange();

network->initBusUpdate();
factory.setYBus();
factory.setMode(YBus);
FullMatrixMap<PFNetwork> mMap(network);
shared_ptr<Matrix> Y = mMap.mapToMatrix();
factory.setSBus();
factory.setMode(SBus);
BusVectorMap<PFNetwork> vMap(network);
shared_ptr<Vector> PQ = vMap.mapToVector();
factory.setMode(Jacobian);
FullMatrixMap<PFNetwork> jMap(network);
shared_ptr<Matrix> J = jMap.mapToMatrix();
shared_ptr<Vector> X(PQ->clone());

double tolerance = 1.0e-6;
int max_iteration = 100;
ComplexType tol = 2.0*tolerance;
LinearSolver isolver(*J);

int iter = 0;
while (real(tol) > tolerance && iter < max_iteration) {
  vMap.mapToBus(X);
network->updateBuses();
factory.setMode(YBus);
factory.setMode(RHS);
  vMap.mapToVector(PQ);
  factory.setMode(Jacobian);
  jMap.mapToMatrix(J);
  LinearSolver solver(*J);
solver.solve(*PQ, *X);
tol = X->norm2();
  iter++;
}

while (real(tol) > tolerance && iter < max_iteration) { 
  vMap.mapToBus(X);
network->updateBuses();
factory.setMode(RHS);
  vMap.mapToVector(PQ);
  factory.setMode(Jacobian);
  jMap.mapToMatrix(J);
  LinearSolver solver(*J);
solver.solve(*PQ, *X);
tol = X->norm2();
  iter++;
}

Figure 3: Top-level driver for a powerflow application using GridPACK™.
Y-matrix. This calculation is triggered by the application-specific setYBus factory method (line 16). Line 17 sets an internal mode in the buses and branches so that they will produce the Y-matrix. The Y-matrix itself is produced by creating a mapper and then using this to generate the matrix (line 18 and 19). The right-hand-side vector for the powerflow equations and the Jacobian are produced in a similar way in lines 21-29.

The next block of code sets up a Newton-Raphson iteration loop. The tolerance and maximum numbers of iterations have been hard-wired in this example but they would be made configurable in an actual application. The code creates a LinearSolver component, based on the current Jacobian, in line 34 and then uses this to get the initial solution to the powerflow equations. The norm of this solution (line 39) is evaluated and if it turns out to be less than the tolerance then the calculation is over (line 41). Otherwise, the solution is pushed back onto the buses (line 43) and the ghost buses are refreshed with current values of the solution (line 44). This data is then used to recalculate the Jacobian and right-hand-side vectors (lines 45-48) and resolved. This process is repeated until the solution converges or the maximum number of iterations is reached. Although the actual working code contains more options for configuring the calculation at runtime, as well as additional options for output, the overall complexity of the driver is about the same as this code fragment.

As mentioned above, most of the code development focuses on creating the bus and branch components, which are responsible for implementing the equations representing the matrix elements in the algebraic equations used to solve the power grid problem. However, because these equations are almost always represented as simple loops over neighbors, they are relatively simple to write. The complexity associated with writing communication routines and performing the index transformations that determine where data comes from and where it goes have been completely abstracted by the framework components.

5. SUMMARY

A schematic of the entire GridPACK™ framework is shown Figure 4. The application-independent modules (in green) have been separated from the application specific modules (in blue). The goal has been to hide as much of the complexity of parallel programming as possible into generic functionality that could be used by multiple applications. A particular focus has been the routines that require extensive communication and/or algorithmic complexity. Successfully encapsulating these into standalone modules that can be used across applications could dramatically reduce the level of effort required to write power grid applications.

As shown in the figure, application developers will need to focus on writing three sets of modules. The network components contain the descriptions of the physics and/or measurements that are associated with buses and branches in the power grid network. The network factory is a module that initializes the grid components on the network after the network is originally created by the import module. The factory can also be used to implement other functions that manage interactions between the network and the network components. The solver is built out of the math module and encapsulates the solution algorithm for the application. Several parallel applications are currently under development using the GridPACK™ and are expected to be completed shortly.

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Figure 4: A schematic diagram of the GridPACK™ framework software layers. Yellow is used for core distributed data objects, green for framework components and blue for application-specific components.
8. REFERENCES


