Lighthouse: A User-Centered Web Service for Linear Algebra Software

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ABSTRACT

Various fields of science and engineering rely on linear algebra for large scale data analysis, modeling and simulation, machine learning, and other applied problems. Linear algebra computations often dominate the execution time of such applications. Meanwhile, experts in these domains typically lack the training or time required to develop efficient, high-performance implementations of linear algebra algorithms. In the Lighthouse project, we enable developers with varied backgrounds to readily discover and effectively apply the best available numerical software for their problems. We have developed a search-based expert system that combines expert knowledge, machine learning-based classification of existing numerical software collections, and automated code generation and optimization. Lighthouse provides a novel software engineering environment aimed at maximizing both developer productivity and application performance for dense and sparse linear algebra computations.

Categories and Subject Descriptors

G.4 [Mathematical Software]: User interfaces; H.4 [Information Systems Applications]: Miscellaneous; D.2.8 [Software Engineering]: Metrics—complexity measures, performance measures

General Terms

Design, Performance

Keywords

web application, user-centered design, data mining, machine learning, taxonomy, linear algebra, mathematical software

1. INTRODUCTION

Scientists and engineers in a wide variety of disciplines rely on linear algebra algorithms (e.g., [22,27,35]) and their high-performance implementations in an ever-expanding field of numerical libraries [1]. Selecting a suitable library and using it effectively to solve a given problem generally require significant background in numerical analysis, high-performance computing (HPC), and software engineering. It also typically involves reading documentation (when available) or researching publications outside of the developer’s area of expertise. Hence, while continuous advances in numerical analysis and HPC libraries allow scientists and engineers to solve larger and more complex problems than ever before, the likelihood that the most relevant and best-performing solution method is identified by each potential user is steadily decreasing.

Linear algebra often constitutes the most time-consuming part of scientific applications’ execution time; therefore, reducing the costs of these computations can have a significant impact on overall software performance. The process of converting linear algebra from base algorithm to high-quality implementation, however, is a complex one. Generally, such transformations require expertise in numerical computation, mathematical software, compilers, and computer architecture and require large, sustained efforts. Current high-performance implementations of numerical linear algebra software are based on decades of applied mathematics research and many thousands of person-hours of effort that is still ongoing. Thus, to optimize both scientific productivity and application performance, an application developer whose problems are too large or complex to solve efficiently through simple sequential algorithms simply cannot afford to develop his or her own HPC implementations and must use HPC libraries developed by others.

Matching numerical capabilities with users’ specific HPC needs is currently not supported by software engineering
tools. With the Lighthouse project, our goal is to provide a structured taxonomy-based interface to high-performance linear algebra software and thereby to enable different types of users to use HPC libraries effectively. We combine taxonomy-based search for identifying specific solution methods with code generation and optimization capabilities to accommodate a variety of different use cases that may arise in HPC software development.

A number of taxonomies exist to aid developers in the translation of linear algebra algorithms to numerical software (e.g., [1, 4, 26, 31]). However, none of these taxonomies provides an accessible interface, nor do they supply tools for high quantity code production. Lighthouse [12] is the first framework that offers a searchable ontology of linear algebra software with code generation and tuning capabilities. Like lighthouses that aid in maritime navigation, our Lighthouse will guide practitioners through the obscure maze of numerical software development. The contributions described in this paper include the following:

- Construction of a software taxonomy that provides an organized anthology of software components for linear algebra.
- Functionality- and performance-based search of high-performance numerical software capabilities with current support for sequential and parallel dense and sparse linear algebra computations provided by the LAPACK [6, 16], PETSc [17–19], and SLEPc [11, 25] libraries.
- Generation of code templates based on search results to automate initial application design.
- Generation of highly tuned code from high-level computation descriptions expressed in a MATLAB-like language.

This paper is organized as follows. Section 2 presents our motivation and related work. Section 3 describes the procedure of developing the Lighthouse taxonomy that covers LAPACK, PETSc, and SLEPc, the strategies for designing the user-centered interfaces that offer effective search functions, and the methods for establishing the support for high-performance implementation. Section 4 discusses the specific implementation approaches for the different numerical packages we have integrated into Lighthouse. Section 5 presents our conclusions and outlines future work.

2. BACKGROUND

A number of taxonomies exist to aid the code developer in translation of linear algebra algorithms to numerical software. Perhaps the oldest one is the Netlib Mathematical Software Repository [4], started in 1985, which contains freely available software, documents, and databases pertaining to numerical computing including linear algebra. Contents are provided as lists of packages or routines, with or without some explanatory words. In newer work, the Linear Algebra Software Survey [24] lists over sixty items categorized as support routines, dense direct solvers, sparse direct solvers, preconditioners, sparse iterative solvers, and sparse eigenvalue solvers together with a checklist specifying problem types for each entry. NIST’s Guide to Available Mathematical Software (GAMS) [31] includes even more basic linear algebra software along with software for a variety of other numerical applications. While the Linear Algebra Software Survey is a linear list, GAMS allows search by problem solved, package name, module name, or text in module abstract. An earlier Java-based client called HotGAMS [30] allowed an interactive search of the GAMS repository. Both the Survey and GAMS index into Netlib for software downloads. Another related taxonomy example not from linear algebra is the decision tree for optimization software at Arizona State University [29]. It refers to Netlib entries if available or points directly to the home page of the software package.

While existing taxonomies represent extensive and valuable resources, the function-level indexing approaches they implement are usually unable to accommodate high-level operations for which no library implementation is available or for which complex software packages, such as PETSc and Trilinos [13], are required. In addition, they serve primarily as references to numerical software collections and require significant linear algebra knowledge to use effectively. Searching for desirable solvers with these taxonomies can be difficult, and little information about the routines is typically returned. For example, as demonstrated in Figure 1, a keyword search of the the Netlib Repository (standard interface) [8] for “solve a system of linear equations general complex” using “any of the words” returns 5581 results containing routines for various purposes, technical reports, conference papers, documentation files, and broken link. Changing this to “all the words” results in no matches even though Netlib does include routines for solving systems of linear equations with dense, complex coefficient matrices. The same keyword search repeated on NIST’s Guide to Available Mathematical Software (GAMS) [31] returns 1,485 largely irrelevant routines. The link for each routine leads to a webpage offering only a small amount of information about that routine. Google and Bing return 3,700,000 and 6,330,000 results, respectively, mostly to non-software related pages.

A final example is the LAPACK Search Engine [26], which provides a simple way to search the list of LAPACK routines. A user enters a problem type (e.g., linear equations or orthogonal factorization), problem parameters (e.g., real, single precision, banded matrix), and the desired operation (e.g., estimate condition number or factor without pivoting). The search engine then either displays the code for the most appropriate routine or allows the user to download it as a zip or tar file. The LAPACK Search Engine provides help with various LAPACK-related language but ultimately delivers only the code itself with no added information about its use.

Lighthouse was inspired by the LAPACK Search Engine. Like the LAPACK Search Engine and unlike the alternatives, Lighthouse typically leads users to a single subroutine. Lighthouse surpasses existing taxonomies in the extent of information available about each routine in the taxonomy, including automatically extracted documentation and additional documentation added manually. Unlike most taxonomy efforts, Lighthouse goes beyond functional classification of software and provides a variety of code generation and optimization capabilities, making it a multi-purpose tool that both educates developers and automates portions of the software design and implementation process for HPC applications.
3. LIGHTHOUSE DESIGN

Lighthouse is an expert system designed to provide four main types of capabilities: (1) functional ontologies of existing numerical software collections; (2) guided, advanced, and keyword-based search for computational routines in the ontologies; (3) generation of code templates based on taxonomy search results; and (4) a high-level scripting interface that accepts input in a high-level MATLAB-like language and generates optimized C implementations. In the remainder of this section, we describe each of these elements.

3.1 Software Classification

A growing number of libraries support linear algebra computations. They include a plethora of specialized algorithms and data structures. To identify the best strategy for reaching the most appropriate and best performing solution for a specific problem, the user answers a series of succinct questions via guided search interfaces for each software package. In each case, the process of answering these questions corresponds to the traversal of a decision tree from root to terminal nodes or leaves. The decision nodes translate into the questions and the terminal nodes indicate or predict target routines. In the remainder of this section we overview the general design and implementation aspects of Lighthouse for LAPACK. Both the interface and internal representation are designed to be easily updatable and extensible for new numerical libraries. For example, the guided search questions corresponding to internal nodes of the decision tree are stored in the database and the web forms in the Lighthouse guided search interface are dynamically generated from that data. Each subsequent question is selected based on the preceding set of responses.

3.2 Search Capabilities and User Interface

The Lighthouse taxonomy information is stored in a MySQL database. The main infrastructure of Lighthouse uses Django [5], an open-source, high-level Python web framework that provides a dynamic database access application programming interface (API). To accommodate users with diverse backgrounds and different programming experiences, Lighthouse provides different levels of user interfaces for subroutine search. For example, through pairing with Haystack [2], Lighthouse enables numerical subroutine search via three methods: guided search, advanced search, and keyword search. In the guided search interface, users are prompted to answer increasingly detailed questions describing the problems they wish to solve. The response to each question triggers a query to the database and directs the search to the most appropriate result. Portions of the interface are automatically generated to display the responses and search results using Django dynamic forms and the Django session framework. Figure 2 shows partial guided search dialogs and the search result. After answering the last question, users typically obtain exactly one routine that matches all of the answers.

Unlike the guided search, the advanced search is designed for users who are familiar with the library. The LAPACK advanced search interface provides users with a form containing checkboxes where they can make multiple selections. The advanced search enables the simultaneous search for multiple routines in different types of functional categories.

The keyword search interface supports subroutine search based on an input keyword or phrase. In order to enhance effectiveness and efficiency, Lighthouse provides automatic completion and spelling correction with words collected from linear algebra textbook indices. In addition, Lighthouse uses a list of linear algebra terms and phrases for Django-Haystack filtering in order to reduce search time. As illustrated in Figure 3, Lighthouse returns five LAPACK routines with keywords “solve a system of linear equations general complex”.

3.3 Code Template Generation

Once a user has identified one or more subroutines through any of the Lighthouse searches, a code template can be generated and downloaded. The template is a complete compilable and runnable program that declares variables using library-specific data structures, initializes them properly, and calls the appropriate subroutine(s) correctly. In addition, each template program is structured into several subprograms, making it easy for users to modify and extend the initial code to fit specific needs.

To generate the templates for LAPACK routines, we first constructed a database that stores the parameters of the subroutines and their types. We then created template base files in both Fortran 90 and C based on several different categories of subroutines. When a user clicks the template gen-

Figure 1: Keyword search “solve a system of linear equations general complex” with Netlib (left) and with GAMS (right).
3.4 Autotuning

Lighthouse provides preliminary support for generating highly optimized code for custom dense linear algebra computations by interfacing with the Build to Order (BTO) [20, 33] compiler. BTO’s input is a MATLAB-like language for defining sequences of basic linear algebra operations. The ability to generate custom optimized implementation of certain linear algebra computations is useful when there is no existing optimized library implementation. BTO performs a number of domain-specific optimizations and employs an empirical autotuning approach to generate a high-performance C implementation of the operations specified by the input. Lighthouse implements a web-based client and corresponding BTO servers running on remote machines. The user inputs the script into the Lighthouse web interface, which provides syntax checking and type inference (types can also be optionally specified explicitly by the user). After verifying (at the client) that the syntax is correct, the code is sent to the BTO server, which then generates different low-level implementations, which are compiled and executed on the remote server to determine the best-performing variant. Because autotuning is most effective when performed on a system similar to that which will be used for production application runs, we will eventually support the use of user-selected servers. The current prototype supports a limited fixed set of servers managed by us.

Figure 5 illustrates the use of Lighthouse and BTO to generate and autotune C code for computing the following
matrix-vector operations:

\[ B = A + u_1 \cdot v_1' + u_2 \cdot v_2' \]
\[ x = b \cdot (B' \cdot y) + z \]
\[ w = a \cdot (B \cdot x) \],

where \( A \) and \( B \) are matrices, \( u_1, u_2, v_1, v_2, w, x, y, \) and \( z \) are vectors, and \( a \) and \( b \) are scalars. The “Input” area in the Lighthouse script section contains two text fields that allow users to input a kernel name and a sequence of linear algebra equations in a high-level MATLAB-like syntax. Once the information is submitted, a list of parameters is dynamically generated including automatic setup of procedure arguments (in, out, inout), data type specifications (scalar, vector, matrix), and orientation declaration (row, column). Users can change these pre-declared values by selecting different options from drop-down lists. When the “Generate Code with BTO” button is clicked, an input file is automatically created and submitted to the server. After the autotuning is complete, the optimized C code is displayed in the “Output” area and can be downloaded by clicking the “Download output file” button. Users can modify and integrate the C code into a larger application context to maximize performance.

4. HPC LIBRARIES

We are continually extending Lighthouse by adding new functionality and improving performance. The currently supported libraries represent an important milestone because they cover a broad space of sequential and parallel solution methods for sparse and dense eigenproblems and systems of linear equations. The Lighthouse application currently offers access to functionality from three linear algebra packages: LAPACK, PETSc, and SLEPc. In the remainder of this section we discuss specific use cases and implementation details for each of the three libraries.

4.1 Lighthouse for LAPACK

LAPACK (Linear Algebra Package) is a large Fortran library for numerical linear algebra. Being one of the most widely used dense direct solver packages for dense matrices, LAPACK was the logical first choice for inclusion in the Lighthouse taxonomy. The Lighthouse taxonomy is continuously expanding and presently contains over 800 LAPACK routines for performing a variety of linear algebra tasks.

The data structures used by LAPACK for different kinds of linear systems play an important role in the decision trees for selecting appropriate subroutines. For example, the linear solver subroutines are first categorized by the kinds of tasks they perform. The system then sorts and identifies eight different matrix types and five different storage methods. Next it categorizes the precision level (single or double) and parameter type (real or complex) of the routines. The database and the step-by-step questions in the guided search abstracted from the decision tree form an effective system for helping users make informed decisions about the most desirable routines. The following use case describes a scenario where a Lighthouse user interacts with the guided search to obtain a single LAPACK linear solver routine.

1. Use Case Name: Searching for an LAPACK routine for solving a system of linear equations.
2. Actors: User, Lighthouse
3. Preconditions: There is an active network connection to Lighthouse; User is at the guided search page of Lighthouse for LAPACK.
4. Basic Flow of Events:
   (a) The use case begins when the guided search page for LAPACK is opened.
   (b) Lighthouse asks “Which of the following functions do you wish to execute?” and displays all the different alternatives that are available on this page.
   (c) User selects “Solve a system of linear equations only” and submits that answer.
   (d) Lighthouse displays resultant routines in the Search Result area and asks “What form of the linear system do you want to solve?”
   (e) User selects “AX = B” and submits the answer.
   (f) Lighthouse updates the search results and asks “Are there complex numbers in your matrix?”
   (g) User selects “No” and submits the answer.
(h) Lighthouse updates the search results and asks “What is the type of your matrix?”
(i) User selects “general” and submits the answer.
(j) Lighthouse updates the search results and asks “How is your matrix stored?”
(k) User selects “band” and submits that answer.
(l) Lighthouse returns the final result, DGBSV, and displays “End of guided search! Check out the result.”
(o) The use case ends successfully.

5. Post-conditions: User has obtained the target LAPACK linear solver routine

In addition to providing the search and code generation capabilities described in Sec. 3, Lighthouse serves as an educational tool. Information about the definition of a word or a phrase, the numerical library, and individual subroutines can be easily accessed by clicking on the help icons or the “more” buttons available throughout the page. Figure 6 shows a pop-up window containing detailed information for a particular subroutine. The intuitive drag-and-drop feature within the Lighthouse interface enables users to simply select a routine by grabbing it and dragging it to the “Selected Routines” work area for code template generation as shown in Figure 4.

Figure 6: A pop-up window displaying subroutine documentation.

Several of the Lighthouse LAPACK code templates contain decision logic to enable tailoring of the solution to specific problem characteristics. For example, code templates for equilibration routines can also determine whether a given matrix is worth scaling. If it is, a method of matrix scaling (row, column, or row-and-column) is automatically selected and executed, and the scaled matrix is returned. The downloadable LAPACK code templates are stored archived for downloading. Each zip file contains a code template file, a README file, and a portable makefile for building on most unix platforms. The README file explains in detail how to best use the template. The makefile helps users compile the code and can be easily modified to suit users’ specific needs.

4.2 Lighthouse for PETSc

For solving large systems of sparse linear equations, Lighthouse provides search and code generation capabilities for the widely used Portable Extensible Toolkit for Scientific Computation (PETSc) [10]. Lighthouse for PETSc has a simple and yet efficient navigation system that enables users to generate, download, and extend complete PETSc-based applications for solving large sparse systems. Specifically, it automates the nontrivial selection of a Krylov subspace (KSP) method and a preconditioner to accelerate convergence rate and reduce execution time. What makes linear solver method selection difficult in practice is that different methods can exhibit very different convergence behavior depending on the (possibly unknown) properties of the linear system and, in many cases, may fail to converge at all. At the time of this writing, PETSc provides more than 20 Krylov subspace methods and over 35 preconditioning methods. The task of selecting “the best” solver-preconditioner combination among the hundreds or thousands of valid pairings and configuring them in a way that maximizes performance is currently left to the application developer who is typically a scientist or engineer whose primary expertise is not in applied mathematics or HPC algorithms. Moreover, for most of these methods, one cannot analytically determine the best algorithms even if all linear system properties are known in advance.

The integration of Lighthouse aims to address two different needs. First, just as they do for dense linear system problems, users interactively express their problem in the way most natural to them, and, based on the user input, Lighthouse generates a complete code template and a set of configuration options that can be used as a starting point for future extensions. Second, Lighthouse tackles the problem of determining what “the best” solution method (KSP solver and preconditioner pair) is for a given linear system. Users have the option of either uploading a sample linear system for Lighthouse to analyze, or they can specify the properties they know directly.

To illustrate how Lighthouse supports solving large sparse linear systems by using PETSc, we describe an example use case.

1. Use Case Name: Solving a large sparse linear system of equations.
2. Actors: User, Lighthouse
3. Preconditions: There is an active network connection to Lighthouse; the user is at the guided search page of Lighthouse for PETSc.
4. Normal flow:
   (a) Lighthouse asks the user if they want to upload their matrix.
   (b) User chooses to upload their matrix.
   (c) Lighthouse provides the user with a file browser for selecting the matrix file.
   (d) User selects the matrix file.
   (e) Lighthouse asks the user if they want a sequential solution or a parallel solution.
   (f) User selects the type of solution they want.
User submits the form.

Lighthouse generates a PETSc program in C programming language, a makefile, a text file containing the command line options and a README file.

Lighthouse then creates an archive file containing the files generated in the previous step.

Lighthouse provides the user with a download link of the archive file.

User downloads the archive file.

Lighthouse deletes user files from the server.

The use case ends successfully.

5. **Post-conditions:** User has obtained an application template and a set of options for configuring the best sparse linear solver and preconditioner for the given linear system.

### 4.2.1 PETSc Search Interface

To implement the PETSc guided search, we began by categorizing matrices based on matrix properties including structural (e.g., symmetry, average or max/min number of nonzeros per row), norm (e.g., 1-, infinity-, and Frobenius norms), spectral (e.g., condition number estimates), normality, and variance (e.g., element variability in rows and columns). Next, we considered a number of use cases [15] to organize and model the interaction between users and Lighthouse. The resultant data set and use cases have suggested that Lighthouse for PETSc provides users with the following options of operation:

1. Compute matrix properties with Lighthouse;
2. Download a PETSc program for computing matrix properties;
3. Download a general PETSc program for solving a linear system;
4. Upload matrix properties computed using the user’s own program.

If option (1) is selected, Lighthouse provides code for the task and a makefile for compiling the code, both of which can be viewed in the respective tabs before downloading. If option (2) is selected, an archive file containing the matrix property computation program and other necessary files is provided. If option (3) is selected as shown in Figure 7, a default PETSc program without a suggestion of a set of a Krylov subspace method and a preconditioner is generated along with other necessary files. Figure 8 illustrates portions of the resulting code template and makefile. This option is for users who are familiar with Krylov methods and know the preconditioner they wish to use. If option (4) is selected, users are guided to answer increasingly detailed questions, and an archive file that includes the program and the files required for the program is delivered at the end of the process.

### 4.2.2 Solver Selection

To select a well-performing method, we must have a way to predict its performance for any valid input. In the case of sparse linear solvers, the inputs are the linear system (matrix) and one or more right-hand side vectors. All of the

Krylov subspace methods in PETSc have the same asymptotic complexity but can differ significantly in their convergence rates for a given linear system. Moreover, the choice of preconditioning method is also very important (there is a tradeoff between computational cost and the accuracy of the inverse approximation produced by a given preconditioner). Because of these complexities (and lack of theoretical models), we modeled the performance of solver/preconditioner methods by using a machine learning approach.

First, we considered a set of 30 linear system properties, including matrix dimension, nonzero statistics, symmetry and other structural characteristics, trace, various norms, dominance, and variance. Because such a large set of features is too expensive to compute during the application’s execution, we applied principal component analysis (PCA) [3] to the data generated by using different solvers to solve 860 real square linear systems obtained from the University of Florida Sparse Matrix Collection [14]. We solved each of these sparse linear system by using different combinations of a Krylov subspace method (including CG, CGS, BICG, BICGSTAB, GMRES, FGMRES, and TFQMR) and a preconditioner (including ILU(k) with different levels of fill, Jacobi, block Jacobi, SOR, and ASM), and evaluated the convergence and the time to solution for each computation. Then we applied PCA by using the MATLAB Statistics Toolbox [28] and identified 15 properties that account for the greatest variability in the data, which enabled us to reduce the feature set from 30 properties to 15 (shown in Table 1). For very long-running simulations, using better-performing solvers quickly amortizes the initial overhead for computing the features needed for selecting the solver and preconditioner.

Second, we explored different machine learning techniques for building a model of the performance based on the set of linear system features, including Naive Bayes classifiers, support vector machines (SVM), alternating decision trees, de-
Figure 8: PETSc search result: Code template and Makefile.

cision stumps, and instance-based learning. For our training set, SVM [23] was consistently more accurate than the other approaches in selecting the best combination of a Krylov subspace method and a preconditioner for any inputs (not in the training set). The average accuracy of the prediction for sequential problems is 85.41% and for parallel problems is 81.95%. As users contribute more linear systems, we will periodically update our training set and update the models to improve the accuracy of the classification for a wider variety of linear systems.

At present we use the classifier to create a single static configuration for a given linear system. In many applications, such as the solution on nonlinear partial differential equations through Newton-Krylov methods, one must solve many sparse linear systems during a single application execution. While some of the linear system properties may remain the same throughout such simulations, others may change, and the initial choice of Krylov method/preconditioner pair may not be the best for all linear systems that arise in a single application run. We plan to integrate some of the adaptive linear solver techniques we have explored previously [21,32] into Lighthouse by generating code templates that allow run-time method selection by periodically computing the properties of selected linear systems and applying the ML-based model to select a different solver/preconditioner combination.

4.3 Lighthouse for SLEPc

Built on top of PETSc, SLEPc is a parallel toolkit for solving large sparse eigenproblems and is the most recent addition to the Lighthouse taxonomy. SLEPc provides six main types of solvers: EPS (Eigenvalue Problem Solver), ST (Spectral Transform), SVD (Singular Value Decomposition), QEP (Quadratic Eigenvalue Problem), NEP (Nonlinear Eigenvalue Problem), and MFN (Matrix Function). Our work has primarily focused on the analysis of the EPS eigensolver routines and their integration into Lighthouse.

To illustrate how Lighthouse supports solving large sparse eigensystems by using SLEPc, we describe an example use case.

1. **Use Case Name:** Searching the SLEPc package for the best eigensolver routine for a sparse matrix.
2. **Actors:** User, Lighthouse
3. **Preconditions:** There is an active network connection to Lighthouse; the user is at the guided search page of Lighthouse for SLEPc.
4. **Basic Flow of Events:**
   a. The guided search page for SLEPc is opened and the series of questions corresponding to the features of the matrix and the result characteristics are displayed.
   b. User answers questions with respect to matrix properties like Hermitian or non-Hermitian, real or complex, etc.
   c. User selects expected properties of the results such as the number of eigenvalues, tolerance desired, portion of eigenvalue spectrum.
   d. User selects available resources such as number of processors available.
   e. Every user selection updates the results matching solvers (e.g., Power, Arnoldi).
   f. Lighthouse returns the final result of best solvers when all questions are answered.
   g. The use case ends successfully.

5. **Post-conditions:** User has obtained the best sparse eigensolver routine(s) with respect to the conditions specified.
Most of the eigensolvers available in SLEPc are compatible with most types of problems. However, not all solvers are equal in terms of accuracy and efficiency. An improper solver selection can result in an unacceptably high residual, lead to essentially no convergence, or yield no feasible solution. By analyzing SLEPc solvers for various input conditions and applying machine learning techniques to the resultant data, we have enabled Lighthouse to identify reliably performant methods for finding eigenvalues and eigenvectors of wide variety of input problems.

Unlike LAPACK linear solvers, where typically there is one solution method that is best suited to a particular problem, there can be multiple SLEPc eigensolver routines providing similar performance and accuracy. Hence, instead of finding a single best solver we look for multiple SLEPc routines that exhibit similar performance for different input cases. To determine the best SLEPc eigensolvers for a given problem, we experimented with compatible routines for various matrices and input parameters using matrices obtained from the University of Florida Sparse Matrix Collection and Matrix Market [7]. Table 2 shows the range of input cases tested, and Table 3 shows the SLEPc solvers run for these input cases. We recorded the statistics of the output characteristics including time to solution, residual, and number of converged eigenvalues. Some of the output characteristics vary substantially with different solvers for the same matrix and input parameters.

Table 2: Input parameters used for eigensolver classification.

<table>
<thead>
<tr>
<th>Property tested</th>
<th>Range of sample tested</th>
</tr>
</thead>
<tbody>
<tr>
<td>Matrix order</td>
<td>112 × 112 to 262111 × 262111</td>
</tr>
<tr>
<td>Matrix type</td>
<td>Real, Complex</td>
</tr>
<tr>
<td>Matrix data</td>
<td>Binary, Double</td>
</tr>
<tr>
<td>Matrix characteristics</td>
<td>Hermitian, Non-Hermitian</td>
</tr>
<tr>
<td>Number of eigenvalues</td>
<td>1, 2, 5, 10</td>
</tr>
<tr>
<td>Portion of spectrum</td>
<td>Largest magnitude, Smallest magnitude, Largest real, Smallest real, Largest imaginary, Smallest imaginary</td>
</tr>
<tr>
<td>Tolerance</td>
<td>1.00E-04, 1.00E-08, 1.00E-10</td>
</tr>
<tr>
<td>Number of processors</td>
<td>1, 2, 4, 8, 12, 24, 48, 96, 192</td>
</tr>
</tbody>
</table>

Table 3: SLEPc solvers in the taxonomy.

| SLEPc solvers | power, subspace, arnoldi, lanczos, krylov schur, generalized davidson, jacobi davidson |

We collected over 29,000 data points and analyzed them with MATLAB to first remove solvers whose number of converged eigenvalues was below the desired value or whose tolerance for the residual was above the threshold. This step gave us a set of eligible solvers. The eigensolver that took the least amount of time was selected as the best fit. In addition, we also identified eigensolvers that take less than 110% of the time taken by the best in order to provide to the users a collection of eigensolvers with similar performance. In 10-fold cross-validation, the average accuracy of predicting the best performing solvers(s) was 86.39%.

These data formed a training set for machine learning to create a model that can make intelligent decisions when selecting solvers for any untested cases. We used MATLAB to implement decision tree induction and adopted ORANGE [9], an open source data mining tool, for generating a classifier in the form of a binary tree as shown in Figure 9. Each node of the tree corresponds to one of the input features such as matrix size, matrix type, and desired eigenvalue spectrum.

Figure 9: A portion of the decision tree for SLEPc.

To integrate the classification tree information into the Lighthouse interface, we converted the decision tree into a MySQL data table using a depth first search algorithm [34]. Every path from the root node to the leaf node forms a single row in the data table. The 395 leaf nodes in the generated decision tree thus resulted in 395 distinct rows with unique features. The user selects the desired features via the Lighthouse-SLEPc interface and the respective best solvers are fetched from the database. The ability to automatically update the decision tree based on new training data ensures that the SLEPc solver recommendations can be improved.

The classification information obtained by using extensive experimentation and machine learning enables Lighthouse to predict the best SLEPc eigensolver for given input and output conditions of a problem. In addition, it provides insight into the design of the guided- and advanced-search interfaces of Lighthouse for SLEPc. Figure 10 illustrates the guided search user interface, consists of a series of simple questions. Answering these questions retrieves the SLEPc eigensolver that works best for the given conditions.

5. CONCLUSION AND FUTURE WORK

This paper describes our work on the development of Light- house, a novel user-centered web service for numerical linear algebra software. The Lighthouse framework comprises a prototype taxonomy of available collections of high-performance numerical software currently including LAPACK, PETSc, and SLEPc. Not only does Lighthouse offer more accurate and robust search capabilities than do the existing taxonomies, it also provides code templates and easy access to the BTO compiler for generating highly tuned implementations of fused linear algebra operations. By following the levels of the decision tree, it identifies the best choice...
of LAPACK routine for dense linear systems. By applying machine learning techniques, Lighthouse is able to suggest a combination of a Krylov subspace method and a preconditioner for a PETSc linear solver with the best expected performance or a set of SLEPc eigensolvers with similar expected performance.

In future work, we will continue to add linear algebra functionality to Lighthouse. In progress now are the inclusion of dense eigensolvers and orthogonal factorizations from LAPACK and sparse linear systems from PETSc. We will also continue to build a complete user interface for each of the existing libraries in Lighthouse. We will also expand the taxonomy and the autotuning support for new types of numerical computations. To take Lighthouse to the next level, we intend to automate the collection and use of performance information in taxonomy searches. We will ultimately provide innovative methods for building a communication platform for cross-domain information exchange on topics related to the contents of the taxonomy.

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6. REFERENCES