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CHAPTER
ONE

INTRODUCTION

This document describes CULA™, an implementation of the Linear Algebra PACKage (LAPACK) interface for CUDA™-enabled NVIDIA® graphics processing units (GPUs).

CULA is a next-generation linear algebra package that uses the GPU as a co-processor to achieve speedups over existing linear algebra packages. CULA provides the same functionality you receive with your existing package, only at a greater speed.

CULA provides easy access to the NVIDIA computing resources available in your computer system. The library is a self-contained package that enhances linear algebra programs with little to no knowledge of the GPU computing model. CULA presents four distinct interfaces:

- **Standard** - The functions in this interface work on data in main memory, as in the Netlib LAPACK interface, but with semantics more familiar to the C and C++ programmer.
- **Device** - This interface follows the standards set forth in the NVIDIA CUBLAS package. In this interface, the user allocates and populates GPU memory and then calls CULA functions to operate on that memory. This is useful for closed-loop GPU systems that do large sections of processing on the GPU.
- **Fortran** - This functions of this interface match the Standard interface but use Fortran calling conventions. The user needs no knowledge of GPU computing, and will feel comfortable if already familiar with LAPACK.
- **Bridge** - This interface is targeted at users who are porting existing linear algebra codes to a GPU-accelerated environment. This interface provides a migration path by matching the function names and signatures of several popular linear algebra packages. It additionally provides a fallback to CPU execution when a user does not have a GPU or when problem size is too small to take advantage of GPU execution.

For maximum compatibility with the conventions of existing linear algebra packages, CULA uses column-major data storage and 1-based indexing, even on our C-oriented interfaces. More details are available in the Programming Considerations chapter.

1.1 Versions

The official release of CULA is available in several forms.

- **Basic** - The basic package contains a basic set of functions and is free of cost. This version supports single-precision real and complex data types.
- **Premium** - The premium package is a low-cost solution that provides a greater set of functionality than the Basic package and includes all data precisions. This package is intended for institutional and academic use.
- **Commercial** - The commercial package contains the functionality of the premium package, but permits the distribution of CULA-powered applications.

The following table summarizes the features of these three versions:
### 1.1.1 Available Functions

CULA implements the most frequently requested functions from LAPACK. As CULA evolves, more functions and function variants will be supported.

CULA Basic contains the following LAPACK function equivalents:

<table>
<thead>
<tr>
<th>Function</th>
<th>Computation Routine</th>
</tr>
</thead>
<tbody>
<tr>
<td>gels</td>
<td>Least squares system solve</td>
</tr>
<tr>
<td>geqrf</td>
<td>QR factorization</td>
</tr>
<tr>
<td>gesv</td>
<td>System solve</td>
</tr>
<tr>
<td>gesvd</td>
<td>Singular value decomposition</td>
</tr>
<tr>
<td>getrf</td>
<td>LU decomposition</td>
</tr>
<tr>
<td>gglse</td>
<td>Constrained least squares system solve</td>
</tr>
</tbody>
</table>

CULA Premium and Commercial support the following functions:

<table>
<thead>
<tr>
<th>Function</th>
<th>Computation Routine</th>
</tr>
</thead>
<tbody>
<tr>
<td>bdsqr</td>
<td>Singular value generation (Bidiagonal)</td>
</tr>
<tr>
<td>gebrd</td>
<td>Bidiagonalization</td>
</tr>
<tr>
<td>gelqf</td>
<td>LQ factorization</td>
</tr>
<tr>
<td>gels</td>
<td>Least squares system solve</td>
</tr>
<tr>
<td>geqrf</td>
<td>QR factorization</td>
</tr>
<tr>
<td>gerqf</td>
<td>RQ factorization</td>
</tr>
<tr>
<td>gesv</td>
<td>System solve</td>
</tr>
<tr>
<td>gesvd</td>
<td>Singular value decomposition</td>
</tr>
<tr>
<td>getrf</td>
<td>LU decomposition</td>
</tr>
<tr>
<td>getri</td>
<td>Matrix inverse</td>
</tr>
<tr>
<td>getrs</td>
<td>LU backsolve</td>
</tr>
<tr>
<td>gglse</td>
<td>Constrained least squares system solve</td>
</tr>
<tr>
<td>ggrqf</td>
<td>Orthogonal matrix factorize (RQ)</td>
</tr>
<tr>
<td>orgbr</td>
<td>Orthogonal matrix generate (Bidiagonal)</td>
</tr>
<tr>
<td>orglq</td>
<td>Orthonormal matrix generate (LQ)</td>
</tr>
<tr>
<td>orgqr</td>
<td>Orthonormal matrix generate (QR)</td>
</tr>
<tr>
<td>ormlq</td>
<td>Orthogonal matrix multiply (LQ)</td>
</tr>
<tr>
<td>ormqr</td>
<td>Orthogonal matrix multiply (QR)</td>
</tr>
<tr>
<td>ormrq</td>
<td>Orthogonal matrix multiply (RQ)</td>
</tr>
<tr>
<td>posv</td>
<td>Symmetric positive definite system solve</td>
</tr>
<tr>
<td>potrf</td>
<td>Cholesky decomposition</td>
</tr>
<tr>
<td>potrs</td>
<td>Cholesky backsolve</td>
</tr>
<tr>
<td>trtri</td>
<td>Triangular matrix inverse</td>
</tr>
<tr>
<td>trtrs</td>
<td>Triangular solve</td>
</tr>
<tr>
<td>ungbbr</td>
<td>Unitary matrix generate (Bidiagonal)</td>
</tr>
<tr>
<td>unglq</td>
<td>Unitary matrix generate (LQ)</td>
</tr>
<tr>
<td>ungqr</td>
<td>Unitary matrix generate (QR)</td>
</tr>
<tr>
<td>unmlq</td>
<td>Unitary matrix multiply (LQ)</td>
</tr>
<tr>
<td>unmqwr</td>
<td>Unitary matrix multiply (QR)</td>
</tr>
<tr>
<td>unmrq</td>
<td>Unitary matrix multiply (RQ)</td>
</tr>
</tbody>
</table>
1.2 Supported Operating Systems

CULA intends to support the full range of operating systems that are supported by CUDA. Installers are currently available for Windows and Linux in 32-bit and 64-bit versions. A 32-bit Mac OS X installer is also available. CULA has been tested on the following systems:

- Windows XP 32 / 64
- Windows Vista 32 / 64
- Ubuntu Linux 9.04
- Red Hat Enterprise Linux 5.3 / 4.7
- Fedora 11
- Mac OS X 10.5 (Leopard) - single precision only. Please see the release notes.

Please provide feedback on any other systems on which you attempt to use CULA. Although we are continually testing CULA on other systems, at present we officially support the above list. If your system is not listed, please let us know through the provided feedback channels.

1.3 Attributions

This work has been made possible by the NASA Small Business Innovation Research (SBIR) program. We recognize NVIDIA for their support.

CULA is built on NVIDIA CUDA 2.3 and NVIDIA CUBLAS.

CULA uses the Intel® Math Kernel Library (MKL) internally. For more information, please see the MKL product page at http://www.intel.com/software/products/mkl.

The original version of LAPACK from which CULA implements a similar interface can be obtained at http://www.netlib.org/lapack.

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This document uses the following notational formats:

- Italic is used for names: CULA.
- Fixed-width is used for code: code.
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8.2 Termination.

1. Breach. Either Party may terminate this Agreement upon thirty (30) days’ prior written notice if the other Party materially breaches this Agreement and does not cure such breach within thirty (30) days following receipt of notice specifying the breach.

2. Insolvency. Either Party may also have the right to terminate this Agreement in the event the other
party (i) becomes insolvent, (ii) becomes subject to a petition in bankruptcy filed by or against it that is not dismissed within thirty days of the filing of such petition, (iii) is placed under the control of a receiver, liquidator or committee of creditors, or (iv) dissolves, ceases to function as a going concern or to conduct its business in the normal course.

8.3 Effect of Termination. Upon the expiration or termination of this Agreement, Customer agrees to pay all amounts accrued or otherwise owing to Licensor on the date of termination, and each Party shall return, or certify the destruction of, the Confidential Information of the other Party. In the event a support program is in place at the effective date of termination, Licensor agrees to continue providing maintenance and support under the terms of this Agreement and the applicable Support Plan through the expiration date of such Support Plan. Termination in accordance with this Agreement shall be without prejudice to any other rights or remedies of the Parties.

9 Miscellaneous.

9.1 Legal Compliance; Restricted Rights. Each Party agrees to comply with all applicable Laws. Without limiting the foregoing, Customer agrees to comply with all U.S. export Laws and applicable export Laws of its locality (if Customer is not located in the United States), and Customer agrees not to export any Network Appliances, Software or other materials provided by Licensor without first obtaining all required authorizations or licenses. The Network Appliances and Software provided to the United States government are provided with only “LIMITED RIGHTS” and “RESTRICTED RIGHTS” as defined in FAR 52.227-14 if the commercial terms are deemed not to apply.

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9.3 Notices. Any notices under this Agreement will be personally delivered or sent by certified or registered mail, return receipt requested, or by nationally recognized overnight express courier, to the address specified herein or such other address as a Party may specify in writing. Such notices will be effective upon receipt, which may be shown by confirmation of delivery. All notices to Licensor shall be sent to the attention of General Counsel (unless otherwise specified by Licensor).

9.4 Assignment. Neither Party may assign or otherwise transfer this Agreement without the other Party’s prior written consent, which consent shall not be unreasonably withheld, conditioned or delayed. Notwithstanding the foregoing, either Party may assign this Agreement without the consent of the other Party if a majority of its outstanding voting capital stock is sold to a third party, or if it sells all or substantially all of its assets or if there is otherwise a change of control. This Agreement shall be binding upon and inure to the benefit of the Parties’ successors and permitted assigns.

9.5 Force Majeure. Neither Party shall be liable for any delay or failure due to a force majeure event and other causes beyond its reasonable control. This provision shall not apply to any of Customer’s payment obligations.

9.6 Counterparts. This Agreement may be executed in counterparts, each of which will be deemed an original, but all of which together will constitute one and the same instrument. This Agreement may be executed by facsimile or scanned signatures.

9.7 General. This Agreement, including its exhibits (all of which are incorporated herein), are collectively the Parties’ complete agreement regarding its subject matter, superseding any prior oral or written communications. Amendments or changes to this Agreement must be in mutually executed writings to be
effective. The individual executing this Agreement on behalf of the Customer has the requisite power and authority to sign this Agreement on behalf of Customer. The Parties agree that, to the extent any Customer purchase or sales order contains terms or conditions that conflict with, or supplement, this Agreement, such terms and conditions shall be void and have no effect, and the provisions of this Agreement shall control. Unless otherwise expressly set forth in an exhibit that is executed by the Parties, this Agreement shall control in the event of any conflict with an exhibit. Sections 2, 3, 5, 6, 7, 8 and 9 and all warranty disclaimers, use restrictions and provisions relating to Licensor’s intellectual property ownership, shall survive the termination or expiration of this Agreement. The Parties are independent contractors for all purposes under this Agreement.

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CULA Basic and CULA Premium Software License Agreement

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CULA Basic Files Re-distributable Pursuant to Section 2.1 (b).

    cula.dll
    cula_fortran.dll
    cula.so.*
    cula_fortran.so.*
    cula.dylib
    cula_fortran.dylib
CHAPTER THREE

GETTING STARTED

3.1 Obtaining CULA

CULA can be downloaded from www.culatools.com. The Basic release is available to those who register on the website. CULA premium, which add dozens of extra LAPACK routines as well as double-precision and double-precision complex data formats, can be purchased from the CULAtools website at www.culatools.com/purchase. For vendors interested in CULA Commercial, please contact EM Photonics directly www.culatools.com/contact.

3.2 System Requirements

CULA utilizes CUDA on an NVIDIA GPU to perform linear algebra operations. Therefore, an NVIDIA GPU with CUDA support is required to use CULA. A list of supported GPUs can be found on NVIDIA’s CUDA Enabled webpage.

Support for double-precision operations requires a GPU that supports CUDA Compute Model 1.3. To find out what Compute Model your GPU supports, please refer to the NVIDIA CUDA Programming Guide.

Note: CULA’s performance is primarily influenced by the processing power of your system’s GPU, and as such a more powerful graphics card will yield better performance.

3.3 Installation

Installation is completed via the downloadable installation packages. To install CULA, refer to the section below that applies to your system.

<table>
<thead>
<tr>
<th>Windows</th>
</tr>
</thead>
<tbody>
<tr>
<td>Run the CULA installer and when prompted select the location to which to install. The default install location is c:\Program Files\CULA. The CULA uninstaller, accessible via the Start Menu, will remove CULA from your system.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Linux</th>
</tr>
</thead>
<tbody>
<tr>
<td>It is recommended that you run the CULA installer as an administrator in order to install to a system-level directory. The default install location is /usr/local/cula.</td>
</tr>
</tbody>
</table>
Mac OS X Leopard

Open the CULA .dmg file and run the installer located inside. The default install location is /usr/local/cula. There is no uninstaller on OS X, but you can remove the folder to which you installed CULA.

Note: You may wish to set up environment variables to common CULA locations. More details are available in the Configuring Your Environment chapter.

3.4 Compiling with CULA

As described in the Introduction, CULA presents four interfaces. This section describes the differences between the Standard and Device interfaces. The third interface (Fortran) is discussed in a later section.

CULA presents two main C headers, culapack.h for the standard interface and culapackdevice.h for the device interface. These files differ in the type of memory they accept. For the Standard interface, the pointers that these functions accept are to main memory, while in Device interface the pointers are to GPU memory. A convenience header cula.h is provided and includes all C functionality.

CULA's Standard interface automatically transfers the contents of the main memory to the GPU before beginning processing, and transfers the results back to the main memory upon completion of the operation. Due to internal memory mechanisms, this can be many times more efficient than allowing the user to pre-load the data to their GPU. However, if the programmer is building a closed-loop GPU system, the data may already be on-card and the CULA Device interface may be more convenient.

CULA's Device interface operates on pre-allocated GPU memory. This interface is intended for those who have pre-existing systems or are trying to build a closed-loop GPU processing system. These inputs are located in GPU memory and the results are placed in GPU memory. Allocation and transfers of data are the responsibility of the programmer and are performed using the CUDA API.

3.5 Linking to CULA

CULA provides a link-time stub library, but is otherwise built as a shared library. Applications should link against the following libraries:

Windows
Choose to link against cula.lib as a link-time option.

Linux / Mac OS X Leopard
Add -lcula to your program's link line.

CULA is built as a shared library, and as such it must be visible to your runtime system. This requires that the shared library is located in a directory that is a member of your system’s runtime library path. For more detailed information regarding operating-system-specific linking procedures, please refer to the Configuring Your Environment chapter.

CULA's example projects are a good resource for learning how to set up CULA for your own project.

Note: CULA is built against NVIDIA CUDA 2.3 and ships with a copy of the CUDA 2.3 redistributable files. If you have a different version of CUDA installed, you must ensure that the CUDA runtime libraries shipped with CULA are the first visible copies to your CULA program. This can be accomplished by placing the CULA bin path earlier in your system PATH than any CUDA bin path. If a non-CUDA-2.3 runtime loads first, you will experience CULA errors.
3.6 Uninstallation

After installation, CULA leaves a record to uninstall itself easily. To uninstall CULA, refer to the section below that applies to your system.

<table>
<thead>
<tr>
<th>Windows</th>
<th>From the Start Menu, navigate to the CULA menu entry under Programs, and select the Uninstall option. The CULA uninstaller will remove CULA from your system.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Linux</td>
<td>Run the CULA installer, providing an ‘uninstall’ argument.</td>
</tr>
<tr>
<td></td>
<td>e.g. ./cula.run uninstall</td>
</tr>
<tr>
<td>Mac OS X Leopard</td>
<td>There is no uninstallation on OS X, but you can remove the folder to which you installed CULA for a complete uninstall.</td>
</tr>
</tbody>
</table>

Note: If you have created environment variables with references to CULA, you may wish to remove them after uninstallation.
CHAPTER
FOUR

DIFFERENCES BETWEEN CULA AND LAPACK

Unlike LAPACK, CULA uses both your system’s CPU and GPU resources. Because of this difference, CULA diverges slightly from the original LAPACK interface. CULA reduces some of the complexities of traditional LAPACK interfaces, while providing the flexibility you need to manage the GPU as a compute device. This section describes the differences between CULA and LAPACK and how they affect your program.

For a discussion on individual routines, see the CULA Reference Manual.

4.1 Naming Conventions

CULA follows a function naming conventions that is similar but different to that of LAPACK. The primary reason for this different is so that the accelerated routines in CULA will be able to link cleanly against other linear algebra packages that supply routines that are not present in CULA. This restriction comes from linkage rules in C/C++ that dictate that there can only be one function of a given name within a program. If CULA used names that are equivalent to those of other packages, this would prevent users from compiling CULA and another linear algebra package in the same program.

CULA’s routines are named using a system where:

• The function begins with cula (in lowercase). Device interface functions use an extended prefix of culaDevice.
• The next character (in uppercase) represents the data type.
• The following two characters (in lowercase) represent the matrix type.
• The final two to three characters (in lowercase) represent the computation performed by the routine.

For example, the following call will perform CULA’s single-precision QR factorization on a general matrix.

\[
\text{culaSgeqrf}
\]

The following table outlines the matrix types specific to CULA.
<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Matrix Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>bd</td>
<td>Bidiagonal</td>
</tr>
<tr>
<td>ge</td>
<td>General</td>
</tr>
<tr>
<td>gg</td>
<td>General matrices, generalized problem</td>
</tr>
<tr>
<td>or</td>
<td>(Real) Orthogonal</td>
</tr>
<tr>
<td>tr</td>
<td>Triangular</td>
</tr>
<tr>
<td>un</td>
<td>(Complex) Unitary</td>
</tr>
</tbody>
</table>

The following table lists the suffix for some common routines CULA provides.

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Computation Routine</th>
</tr>
</thead>
<tbody>
<tr>
<td>trf</td>
<td>Compute a triangular factorization</td>
</tr>
<tr>
<td>sv</td>
<td>Factor the matrix and solve a system of equations</td>
</tr>
<tr>
<td>qrf</td>
<td>Compute a QR factorization without pivoting</td>
</tr>
<tr>
<td>svd</td>
<td>Compute the singular value decomposition</td>
</tr>
<tr>
<td>ls</td>
<td>Solve over- or under-determined linear system</td>
</tr>
</tbody>
</table>

The full list of abbreviations can be found at the LAPACK website.

### 4.2 Calling Conventions

In addition to using different function names, CULA has moved away from the LAPACK interface and takes arguments by value rather than by reference, which is a convention more familiar to C/C++ programmers. Additionally, this simplifies calling code by reducing the need for some temporary variables.

For example, compare a call to a CULA function with one that uses traditional LAPACK conventions:

// Common variables
...

// CULA
culaStatus s;
s = culaSgesvd('O', 'N', m, m, a, lda, s, u, ldu, vt, ldvt);

// Traditional
char jobu = 'O';
char jobvt = 'N';
int info;
sgesvd(&jobu, &jobvt, &m, &m, a, &lda, s, u, &ldu, vt, &ldvt, &info);

Compared to the traditional code, CULA uses fewer lines, has a shorter call line, and is no less clear than the traditional usage – one might argue that it is even more clear because there is less code to inspect.

In addition to the Standard and Device interfaces, CULA has a third interface, Fortran, intended to be used in Fortran programs. This interface follows the conventions of Fortran programming by taking all parameters by reference rather than by value. For more information on this interface, see the ‘fortran_interface.txt’ document in the ‘doc’ directory.

With version 1.1, CULA introduced the Bridge interface. This interface is targeted at users who are porting existing linear algebra codes to a GPU-accelerated environment. The Bridge interface provides a migration path by matching the function names and signatures of several popular linear algebra packages. It additionally provides a fallback to CPU execution when a user does not have a GPU or when problem size is too small to take advantage of GPU execution. For more information on this interface, see the ‘bridge_interface.txt’ document in the ‘doc’ directory.
4.3 Data Type Support

Different versions of CULA support different data types. CULA Basic supports both single-precision real and complex. CULA Premium and Commercial support all LAPACK data types.

CULA provides support for float and float-complex data types by using C’s built-in `float` and the CULA type `culaFloatComplex`. Similarly, CULA provides support for double and double-complex data types by using C’s built-in `double` and the CULA type `culaDoubleComplex`, though these data types require support from the GPU (see System Requirements).

<table>
<thead>
<tr>
<th>Prefix</th>
<th>Data Type</th>
<th>CULA Standard Interface Type</th>
<th>CULA Device Interface Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>S</td>
<td>Single Precision Real</td>
<td><code>culaFloat</code></td>
<td><code>culaDeviceFloat</code></td>
</tr>
<tr>
<td>C</td>
<td>Single Precision Complex</td>
<td><code>culaFloatComplex</code></td>
<td><code>culaDeviceFloatComplex</code></td>
</tr>
<tr>
<td>D</td>
<td>Double Precision Real</td>
<td><code>culaDouble</code></td>
<td><code>culaDeviceDouble</code></td>
</tr>
<tr>
<td>Z</td>
<td>Double Precision Complex</td>
<td><code>culaDoubleComplex</code></td>
<td><code>culaDeviceDoubleComplex</code></td>
</tr>
</tbody>
</table>

Note: CUDA complex types may be used in place of CULA types by defining the preprocessor macro `CUDA_USE_CUDA_COMPLEX` before including a CULA header.

4.4 Error Handling

LAPACK’s error handling is accomplished through an `info` parameter. Upon return, this parameter specifies whether or not the function succeeded (return value of 0) and if it did not, indicates the particular parameter that is in error by stating the parameter number. Additionally, LAPACK may print an error to `stdout`.

CULA uses a system similar to LAPACK’s error handling but adds additional functionality. Instead of requiring an `info` parameter, CULA returns the success or failure of a function using a `culaStatus` enumeration. This return code specifies conditions that the `info` parameter does not cover, including:

- a valid co-processing device is not available;
- insufficient memory is available to continue;
- a requested feature is not available;
- the co-processing device is missing a required feature to complete the requested operation.

Two classes of errors that are typically reported by LAPACK are those in arguments passed to a function and those resulting from malformed data. CULA reports these errors using `culaArgumentError` and `culaDataError` return values. When this value is returned, further information about this error can be requested by calling `culaGetErrorInfo`, which returns an integer equivalent to that which would be returned by the analogous LAPACK function. Unlike LAPACK, CULA will not print information to `stdout`.

4.5 Workspaces

Many LAPACK functions require a workspace for internal operation. For those LAPACK functions that utilize a workspace, workspace sizes are queried by providing a -1 argument to what is typically an `LWORK` parameter. Upon inspecting this parameter, the LAPACK function will determine the workspace required for this particular problem size and will return the value in the `WORK` parameter. LAPACK (and other similar packages) then require the programmer to provide a pointer to memory of sufficient size, which often requires that the programmer allocate new memory.

CULA uses both main and GPU workspace memories, and as such, LAPACK’s workspace query is not appropriate, as the LAPACK interface allows for the specification of only one workspace. Instead of providing a more complicated interface that adds parameters for both main and GPU workspace memories, CULA requires neither. Instead, any
workspaces that are required are allocated and tracked internally. This organization yields no significant performance loss, and furthermore reduces the number of function calls by removing the need for a workspace query.

**Note:** Any workspaces that have been allocated internally may be cleared by calling `cudaFreeBuffers()`.
This chapter contains a variety of subjects related to programming using CULA.

5.1 Matrix Storage

When providing data to CULA routines, it is important to consider the manner in which the data is stored in memory. In particular, there are two important requirements to ensure correct results:

- Data must be in “column-major” order.
- Complex data must be interleaved.

The following sections will briefly explain these requirements.

5.1.1 Column-Major Ordering

CULA routines expect that any data provided will be stored in column-major order. While this storage scheme is also expected for LAPACK routines, column-major order may be uncommon to many programmers. Consider the following M-by-N matrix.

When storing the matrix in memory, two methods are frequently used: row-major and column-major.

For many C programmers, a familiar storage pattern would involve storing the elements of a particular row first, followed by the elements of successive rows. In this storage scheme, elements of a row are contiguous in memory, while elements of a column are not. C, for example, is row-major storage by default.
Column-major ordering is the opposite of this because elements of the matrix are now stored by column, rather than by row. In this storage scheme, elements of a column are contiguous in memory, while elements of a row are not.

As mentioned previously, CULA expects data to be represented in column-major order. Performing a transpose on the row-major data will convert it to column-major and vice-versa.

**Note:** Many CULA functions take a “leading dimension” argument after matrix arguments. For column-major data, the leading dimension is equal to the length of a column, or equivalently, the number of rows in the matrix. This is the length of the allocated memory and may be larger than the memory involved in a particular computation. For submatrix operations or pitched allocations, remember to report the leading dimension parameter as the number of *allocated* rows in the matrix.

**Note:** Note the differences in addressing row-major and column-major order.

Given an element of matrix A (with leading dimension LDA) located at row “i” and column “j,” this element would be accessed as follows:

- $A[j \times LDA + i]$ for row-major data.
- $A[i \times LDA + j]$ for column-major data in CULA.
5.1.2 Complex Data Types

When working with complex data, CULA expects real and complex portions of the matrix to be interleaved. In other words, for any particular element, the real and complex parts are adjacent in memory, with the complex part being stored after the real part.

![Complex Element](image)

Figure 5.4: This figure shows the packing of a complex data element. In memory, the real part of an element is directly followed by the complex component of that element.

5.2 Optimizing for Performance

CULA is specifically designed to leverage the massively parallel computational resources of the GPU, with a particular focus on large problems whose execution on a standard CPU is too time consuming. As such, several considerations should be taken into account when applying CULA routines to maximize overall performance gains.

5.2.1 Problem Size

Prior to the application of CULA routines it is important to consider problem size. As a general rule, applying CULA for larger problems will maximize performance gains with respect to other computational linear algebra packages. For example, consider the SGEQRF Speedups Figure.

![SGEQRF Speedup vs MKL](image)

Figure 5.5: This figure shows the speedup for a selected routine versus problem size. High speedups are attained for larger problem sizes.

The speedup chart illustrates the performance of CULA's QR decomposition with respect to Intel’s Math Kernel Library (MKL). Note that for the smallest problem sizes, no performance gains are seen; however, problem complexity quickly scales in such a manner that the GPU is able to outperform the CPU, for even modest problem sizes.
Note: The maximum problem size is constrained by the data type in use and the maximum GPU memory. For example, the maximum size for a problem that uses double-precision complex data is roughly one fourth of the maximum problem size of a single-precision problem for the same matrix dimensions, since the size of these data types differ by a factor of four.

5.2.2 Accuracy Requirements

CULA offers both single and double-precision floating point support for its included routines. While the latest NVIDIA GPU hardware offers support for both of these data types, it should be noted that current NVIDIA GPU hardware performs best when operating on single-precision data.

When applying CULA routines, the accuracy requirements of the program should be evaluated. If extended precision is required, then the use of double-precision routines is advised. For programs with more relaxed accuracy requirements, however, additional performance can be achieved at the cost of accuracy through the use of single-precision routines.

5.3 Using the Device Interface

CULA’s device interface allows a user to directly control GPU memory. This is useful for closed-loop GPU systems that do large sections of processing on the GPU. The device interface is not recommended to those without CUDA experience.

When using the device interface, include culapackdevice.h instead of culapack.h; see the Matrix Storage section for differences in naming conventions between the Standard and Device interfaces. Memory allocation is handled via cudaMalloc and cudaFree, available in the CUDA toolkit. If the programmer uses pitched memory, it is up to that programmer to ensure that their allocations are appropriate.

Note: CULA’s Premium version provides specialized allocation functions that pitch data to the optimal size for CULA. These functions are culaDeviceMalloc() and culaDeviceFree(), found in the culadevice.h header of CULA Premium.

5.4 Thread Safety/Multi-GPU Operation

Currently, the default operating mode of CULA is to operate on only one GPU. Aside from this default mode, a programmer can manually control the way that CULA is used across the various GPU devices in their system. For a given function call, CULA currently supports single-GPU operation only. However, function calls may be made from several threads because all API functions are designed to be thread safe. Thus, you may write a program that is multithreaded, with various threads making accesses to CULA to perform their individual linear algebra operations.

By default, CULA binds to the best GPU in a system. However, this binding may be manually controlled by using culaSelectDevice (found in culadevice.h). It is important to note that if a given thread is already bound to a particular GPU device, CULA cannot reset this binding, as this is a restriction of CUDA.

To use multiple GPUs, multiple threads must be created. Each thread must be bound to a different GPU device by calling culaSelectDevice, with a different GPU id for each thread. After doing so, call culaInitialize in each thread, and proceed to call CULA functions as you need. Before each thread exits, ensure that culaShutdown is called in each.

When using CULA, normal parallel programming rules apply. The section below outlines a few of these considerations for each of CULA’s interfaces.

<table>
<thead>
<tr>
<th>Standard / Fortran Interface</th>
</tr>
</thead>
<tbody>
<tr>
<td>The Standard interface uses (traditional) main memory pointers. It is up to the programmer to ensure that CULA does not concurrently write to overlapping sections of memory; doing so will yield undefined results.</td>
</tr>
</tbody>
</table>
Device Interface

The CUDA programming model specifies that a given thread may only communicate with a single GPU in a system. To follow this requirement, any call to a CUDA API function or a CULA function will “bind” that thread to that GPU (except where specified). These calls include memory allocations functions. A device pointer is only valid on a particular GPU, so care must be taken when calling CULA in a multithreaded environment. The important point is to only pass device pointers that were allocated in that particular thread context. To learn which device a thread is bound to, you may call culaGetExecutingDevice() routine found in culadevice.h.

5.5 Developing in C++

CULA provides a set of generic functions for use in C++ applications. These functions are overloaded to select a function according to the data type of its operand, allowing generic code. For every function in the culapack.h and culapackdevice.h headers, there is a generic version of that function in the culapack.hpp and culapackdevice.hpp headers. The generic functions will determine the type of the calling data and dispatch the operation to the appropriate typed function. Similarly to the C interfaces, a cula.hpp file is provided as a convenience header to include both the Standard and Device interfaces simultaneously if desired.

Please see the Examples chapter for an example of this interface.
The CULA installation contains several examples that show how to use CULA. These examples are contained in the ‘examples’ directory.

This section lists several of the common use cases for CULA functions.

### 6.1 Initialization and Shutdown

```c
#include <cula.h>

culaStatus s;

s = culaInitialize();
if(s != culaNoError)
{
    printf("%s\n", culaGetErrorString(s));
    /* ... Error Handling ... */
}
/* ... Your code ... */
culaShutdown();
```

### 6.2 Argument Errors

```c
#include <cula.h>

culaStatus s;

s = culaSgeqrf(-1, -1, NULL, -1, NULL); /* obviously wrong */
if(s != culaNoError)
{
    if(s == culaArgumentError)
        printf("Argument %d has an illegal value\n", culaGetErrorInfo());
    else
        printf("%s\n", culaGetErrorString(s));
}
6.3 Data Errors

```c
#include <cula.h>

float *A = malloc(20*20*sizeof(float));
memset(A, 0, 20*20*sizeof(float)); /* singular matrix, illegal for LU (getrf) */
int ipiv[20];
s = culaSgetrf(20, 20, A, 20, ipiv);
if( s !=culaNoError )
{
    if( s ==culaDataError )
        printf("Data error with code %d, please see LAPACK documentation\n",
                culaGetErrorInfo());
    else
        printf("%s\n", culaGetErrorString(s));
}
```

6.4 Using the C++ Interface

```cpp
#include <cula.hpp>

template<class T>
void GenericLU(T *A, int N) // type of T will be determined by the compiler
{
    std::vector<int> piv(N);
    // no need for type specifier - determined automatically on overloads
    culaStatus s = culaGetrf(N, N, A, N, &ipiv[0]);
    // check errors
}
```
CHAPTER
SEVEN

CONFIGURING YOUR ENVIRONMENT

This section describes how to set up CULA using common tools, such as Microsoft® Visual Studio®, as well as command line tools for Linux and Mac OS X.

7.1 Microsoft Visual Studio

This section describes how to configure Microsoft Visual Studio to use CULA. Before following the steps within this section, take note of where you installed CULA (the default is C:\Program Files\CULA). To set up Visual Studio, you will need to set both Global- and Project-level settings. Each of these steps is described in the sections below.

7.1.1 Global Settings

When inside Visual Studio, navigate to the menu bar and select Tools > Options. A window will open that offers several options; in this window, navigate to Projects and Solutions > VC++ Directories. From this dialog you will be able to configure global executable, include, and library paths, which will allow any project that you create to use CULA.

The table below specifies the recommended settings for the various directories that the VC++ Directories dialog makes available. When setting up your environment, prepend the path of your CULA installation to each of the entries in the table below. For example, to set the include path for a typical installation, enter C:\Program Files\CULA\include for the Include Files field.

<table>
<thead>
<tr>
<th>Option</th>
<th>Win32</th>
<th>x64</th>
</tr>
</thead>
<tbody>
<tr>
<td>Executable Files</td>
<td>bin</td>
<td>bin64</td>
</tr>
<tr>
<td>Include Files</td>
<td>include</td>
<td>include</td>
</tr>
<tr>
<td>Library Files</td>
<td>lib</td>
<td>lib64</td>
</tr>
</tbody>
</table>

With these global settings complete, Visual Studio will be able to include CULA files in your application. Before you can compile and link an application that uses CULA, however, you will need to set up your project to link CULA.

7.1.2 Project Settings

To use CULA, you must instruct Visual Studio to link CULA to your application. To do this, right-click on your project and select Properties. From here, navigate to Configuration Properties > Linker > Input. In the Additional Dependencies field, enter “cula.lib”.

On the Windows platform, CULA’s libraries are distributed as a dynamic link library (DLL) (cula.dll) and an import library (cula.lib), located in the bin and lib directories of the CULA installation, respectively. By Linking cula.lib, you are instructing Visual Studio to make an association between your application and the CULA DLL, which will allow your application to use the code that is contained within the CULA DLL.
7.1.3 Runtime Path

CULA is built as a dynamically linked library, and as such it must be visible to your runtime system. This requires that cula.dll and its supporting dll’s are located in a directory that is a member of your system’s runtime path. On Windows, you may do one of several things:

1. Add CULA_BIN_PATH_32 or CULA_BIN_PATH_64 to your PATH environment variable.
2. Copy cula.dll and its dll’s to the working directory or your project’s executable.

7.2 Linux / Mac OS X - Command Line

On a Linux system, a common way of building software is by using command line tools. This section describes how a project that is command line driven can be configured to use CULA.

7.2.1 Configure Environment Variables

The first step in this process is to set up environment variables so that your build scripts can infer the location of CULA.

On a Linux or Mac OS X system, a simple way to set up CULA to use environment variables. For example, on a system that uses the bourne (sh) or bash shells, add the following lines to an appropriate shell configuration file (e.g. .bashrc).

```sh
export CULA_ROOT=/usr/local/cula
export CULA_INC_PATH=$CULA_ROOT/include
export CULA_BIN_PATH_32=$CULA_ROOT/bin
export CULA_BIN_PATH_64=$CULA_ROOT/bin64
export CULA_LIB_PATH_32=$CULA_ROOT/lib
export CULA_LIB_PATH_64=$CULA_ROOT/lib64
```

(where CULA_ROOT is customized to the location you chose to install CULA)

After setting environment variables, you can now configure your build scripts to use CULA.

**Note:** You may need to reload your shell before you can use these variables.

7.2.2 Configure Project Paths

This section describes how to set up the gcc compiler to include CULA in your application. When compiling an application, you will typically need to add the following arguments to your compiler’s argument list:

<table>
<thead>
<tr>
<th>Item</th>
<th>Command</th>
</tr>
</thead>
<tbody>
<tr>
<td>Include Path</td>
<td>-I$CULA_INC_PATH</td>
</tr>
<tr>
<td>Library Path (32-bit arch)</td>
<td>-LCULA_LIB_PATH_32</td>
</tr>
<tr>
<td>Library Path (64-bit arch)</td>
<td>-LCULA_LIB_PATH_64</td>
</tr>
<tr>
<td>Libraries to Link against</td>
<td>-lcuda</td>
</tr>
</tbody>
</table>

For a 32-bit compile:

```
gcc ... -I$CULA_INC_PATH -LCULA_LIB_PATH_32 -lcuda -lcublas -lcudart ...
gcc ... -L$CULA_LIB_PATH_32 -lcuda ...
```

For a 64-bit compile (not applicable to Mac OS X):
gcc ... -I$CULA_INC_PATH -L$CULA_LIB_PATH_64 -lcuda -lcublas -lcudart ... 

7.2.3 Runtime Path

CULA is built as a shared library, and as such it must be visible to your runtime system. This requires that CULA’s shared libraries are located in a directory that is a member of your system’s runtime library path. On Linux, you may do one of several things:

1. Add CULA_LIB_PATH_32 or CULA_LIB_PATH_64 to your LD_LIBRARY_PATH environment variable.

2. Edit your system’s ld.so.conf (found in /etc) to include either CULA_LIB_PATH_32 or CULA_LIB_PATH_64.

On the Mac OS X platform, you must edit the DYLD_LIBRARY_PATH environment variable for your shell, as above.
This section lists solutions for common problems encountered when using CULA and describes your support options.

### 8.1 Common Issues

**How do I report information about my system?**

Run one of the `sysinfo.bat` or `sysinfo.sh` scripts, for Windows or Linux/Mac OS X systems, respectively. The information these scripts report can be uploaded as an attachment to your support requests or forum posts and will aid us greatly in diagnosing your problems.

**`cuda.dll` or `libcula.so` could not be found**

Your runtime system has not been set up to locate CULA. See the Linking to CULA section.

**CULA returns `culaArgumentError`**

Your input to one of CULA's routines is incorrect. The faulty parameter is reported by `culaGetErrorInfo`; ensure that all of your parameters are correct. See the Error Handling section.

**CULA returns `culaDataError`**

An input to one of CULA's routines is malformed or singular. More information about the error is reported by `culaGetErrorInfo`. See the Error Handling section.

**CULA returns `culaRuntimeError`**

The most common cause of this error is related to improperly configured or old GPU drivers. Ensure that your system is up to date by installing the latest drivers from NVIDIA.

If the problem persists, please file a bug report.

**An LAPACK routine I need is missing. What should I do?**

LAPACK is a very large library and we have only written a subset of its capabilities so far. CULA Premium and CULA Commercial are constantly growing as new functions are added. If there is function you would like to see added, contact us on our forums and voice your opinion on which functions you use.

**I’m having problems with my GPU and/or video drivers. Can you help?**

Problems specific to GPU devices and their drivers should be handled by NVIDIA. The latest drivers can always be obtained directly from NVIDIA on their Download page. CULA requires CUDA 2.3 compatible drivers (or newer) to be installed on your system. On Linux, this requires driver version 190.18 or newer, and for Windows it is version 190.38 or newer. On Mac OS X, please use “cudadriver_2.3.0_macos.pkg” or newer.
I think I found a bug. What should I do?

First, be sure that you are experiencing a software bug and not an issue related to faulty hardware or drivers. If you are still reasonably sure you have encountered a bug.

8.2 Support Options

If none of the entries above solve your issue, you can seek technical support. See your license level below to learn about your support options.

- **Basic** - Basic users may post problems to the CULA forums for community support.
- **Premium** - Premium users can submit support tickets through the CULA website to receive personalized help.
- **Commercial** - Commercial users have direct support. Please contact your support representative directly for help with your issue.

When reporting a problem, make sure to include the following information:

- System Information (see *Common Issues*)
- CULA Version
- Version of NVIDIA® CUDA Toolkit installed, if any
- Problem Description (with code if applicable)
CHAPTER
NINE

CHANGELOG

9.1 Release 1.1 Final (November 25, 2009)

All Versions

• Improved: Removed culaInitialize() delay
• Improved: GEQRF performance up to 20% improvement for users with older CPUs
• Fixed: Correction to Fortran example Makefile to specify “arch” parameter

Basic

• Improved: SVD significant memory usage reduction
• Improved: GELS stability for N > M case

Premium

• Improved: GELQF performance increase 2-3x
• Improved: GEHRD/GERQF/ORGLQ/ORGQR performance increased by 10-20%
• Improved: GEHRD routine accurate for size N==1

9.2 Release 1.1 Beta (November 13, 2009)

All Versions

• Feature: Mac OS X 10.5 Leopard “preview” release - single precision only
• Feature: New “Bridge” interface provides for easy and seamless porting of existing LAPACK/MKL/ACML applications (see doc/bridge_interface.txt)
• Feature: New document describing full CULA API
• Feature: New function culaSelectDevice to set executing device
• Feature: New “gesv” example shows operation of all S/C/D/Z data types
• Feature: New “multigpu” example showing multi-GPU CULA operation
• Feature: New “bridge” example showing usage of the Bridge interface
• Improved: SVD optimized for non-square cases
• Improved: Documentation clarified on error conditions and codes
• Improved: Stronger error reporting from example projects
• Improved: cudaInitialize detects and reports if driver/runtime version are inadequate
• Improved: Documentation clearer on thread safety issues
• Fixed: CULA can now handle extremely non-square matrices (e.g., 500000x16)
• Fixed: An error in the “benchmark” example causing it to ignore user arguments
• Fixed: Properly reporting cudaErrorMemoryValueTooLarge as culaInsufficientMemory

Basic
• Improved: GESV performance increased by up to 30%
• Improved: Stability of GELS in certain cases
• Improved: Stability of SVD in certain cases

Premium
• Feature: Implemented geev (general Eigensolver) in S/D/C/Z precisions
• Feature: Implemented gehrd (general Hessenberg reduction) in S/D/C/Z precisions
• Feature: Implemented orghr
• Feature: .hpp headers have name overloads of ORG/UNG functions
• Fixed: Host interface “ORG” functions different results from device interface

9.3 Release 1.0 Final (September 30, 2009)

Basic
• Feature: All functions feature complex variants
• Fixed: Crash related to getrs pivot array

Premium
• Feature: All functions implemented in all supported data types

9.4 Release 1.0 Beta 3 (September 15, 2009)

All Versions
• Feature: New documentation section on specific routine conventions
• Improved: Updated sysinfo script with more descriptive output
• Improved: Added example that demonstrates the device interface
• Fixed: Various corrections for small-matrix inputs, especially M=N=1
• Fixed: cudaInitialize now sets environment variable KMP_DUPLICATE_LIB_OK

Basic
• Feature: Complex geqrf included
• Feature: Added culaGetDeviceCount to report the number of available devices
• Feature: Added culaGetDeviceInfo to report information about a device
• Feature: Added culaGetExecutingDevice to report the executing device
• Fixed: Further corrections for unitary output in gesvd for all job codes

**Premium**
• Feature: New functions culaDeviceMalloc/culaDeviceFree in culadevice.h
• Fixed: Orglq and orgqr should behave more reliably

### 9.5 Release 1.0 Beta 2 (August 27, 2009)

**All Versions**
• Feature: Including both 32- and 64-bit libraries on 64-bit Linux release
• Feature: Now shipping precompiled Benchmark example on Linux builds
• Feature: Troubleshooting section added to Programmer’s Guide
• Feature: Added scripts that report system information to examples folder
• Improved: Error output for examples is now more descriptive
• Improved: Documentation is more specific about configuring system runtime
• Fixed: Incompatibilities with gcc 4.2 and earlier; gcc 4.1 is now compatible

**Basic**
• Improved: gesvd was optimized for up to a 60% speedup over Beta 1
• Fixed: Error in geqrf for matrices of M << N
• Fixed: Error in gesvd where some matrices would yield non-unitary U and Vt

**Premium**
• Feature: Implemented getri
• Feature: Implemented potrf
• Feature: Implemented potrs
• Feature: Implemented posv
• Feature: Implemented trtrs
• Improved: orglq was optimized for up to a 700% speedup

### 9.6 Release 1.0 Beta 1 (August 13, 2009)

**All Versions**
• Feature: Support Windows XP 32/64
• Feature: Support Linux 32/64

**Basic**
• Feature: Implemented gels
• Feature: Implemented geqrf
• Feature: Implemented gesv
• Feature: Implemented gesvd
• Feature: Implemented getrf
• Feature: Implemented gglse

Premium
• Feature: Implemented gebrd
• Feature: Implemented getrs
• Feature: Implemented trtrs
• Feature: Implemented gelqf
• Feature: Implemented gerqf
• Feature: Implemented orgqr
• Feature: Implemented orglq
• Feature: Implemented orgbr
• Feature: Implemented ormqr
• Feature: Implemented ormlq
• Feature: Implemented ormrq
• Feature: Implemented bdsqr