Library Additions and Improvements

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Chapel version 1.18

September 20, 2018

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Outline

- **New Modules**
  - HDF5 Package Module
  - NetCDF Package Module
- **Module Improvements**
  - LinearAlgebra Package Module
  - Crypto Package Module
  - Error-Handling in Standard Modules

New Modules

HDF5 Package Module

HDF5: Background

- **HDF5 is a popular data storage format**
  - "Flexible and efficient I/O and high volume, complex data"
  - Widely used in scientific codes
- **Library is written in C**
- **Chapel should be able to read and write HDF5 files**

HDF5: This Effort

- **Provide an interface for reading/writing HDF5 files**
  - Call HDF5 functions using 'extern's in the 'C_HDF5' sub-module

```
use HDF5.C_HDF5;
// Open the file, read the 64-bit integers into array 'data'
var data: [0..#numElements] int;
const fid = H5open("data.h5", H5F_ACC_RDONLY, H5P_DEFAULT);
H5LTread_dataset(fid, c"dset", H5T_STD_I64LE, c_ptrTo(data));
H5Fclose(fid);
```

- **Provide higher-level functions for reading/writing files**
  - Higher-level functions are in the main 'HDF5' module
    - Read data in chunks
    - Support distributed arrays
    - Apply user-defined preprocessing
    - In parallel

HDF5:

- Example – Reading Block and Cyclic distributed arrays

```
use HDF5, BlockDist, CyclicDist;

const Space = {1..100};
const BlkSpace = Space dmapped Block(boundingBox=Space),
      CycSpace = Space dmapped Cyclic(startIdx=Space.low);

var BlkArr: [BlkSpace] int, CycArr: [CycSpace] int;

hdf5ReadDistributedArray(BlkArr, fileName, blkDsetName);
hdf5ReadDistributedArray(CycArr, fileName, cycDsetName);
```

Regular distributed domain/array declarations

Single function to read arrays for multiple distributions

HDF5: Status and Next Steps

Status:

- HDF5 library is available to call from Chapel
- Several routines written in Chapel to extend the functionality
  - Parallel reads/writes
  - Chunked reads
  - Reads to distributed arrays
  - Preprocessing capabilities

Next Steps:

- Continue to extend the functionality in Chapel
  - Support writes in the same ways as reads
  - Support more distributions
  - Support more file access patterns

NetCDF Package Module

NetCDF

Background: NetCDF is a popular data storage format

- For "creation, access, and sharing of array-oriented scientific data"

This Effort: Provide an interface for reading/writing NetCDF files

- Create 'extern' functions to enable calling the C library from Chapel

```
config const filename = "data.nc";
var ncid, varid: c_int, data: [1..NX, 1..NY] c_int;
nc_open(filename.c_str(), NC_NOWRITE, ncid); // open file for reading
nc_inq_varid(ncid, c"data", varid);          // get the ID for "data"
nc_get_var_int(ncid, varid, data[1,1]);      // read values for "data"
nc_close(ncid);                              // close the file
```

Impact: Chapel programs can now read and write NetCDF files

Next Steps: Create functions for more convenient access to data

- e.g., parallel/distributed reads/writes, data preprocessing capabilities

Module Improvements

LinearAlgebra Package Module

LinearAlgebra: Background

- **Provides a high-level interface for linear algebra**
  - Design influenced by NumPy and MatLab
  - Provides helper functions for creating matrices and vectors as arrays
  - Supports many linear algebra operations on matrices and vectors
- **Implementations use both Chapel and external libraries**
  - Some examples:
    - Dot product (Chapel)
    - Matrix-matrix multiplication (BLAS)
    - Cholesky decomposition (LAPACK)
- **'Sparse' submodule supports sparse linear algebra**
  - Supports a subset of the features available in Linear Algebra module

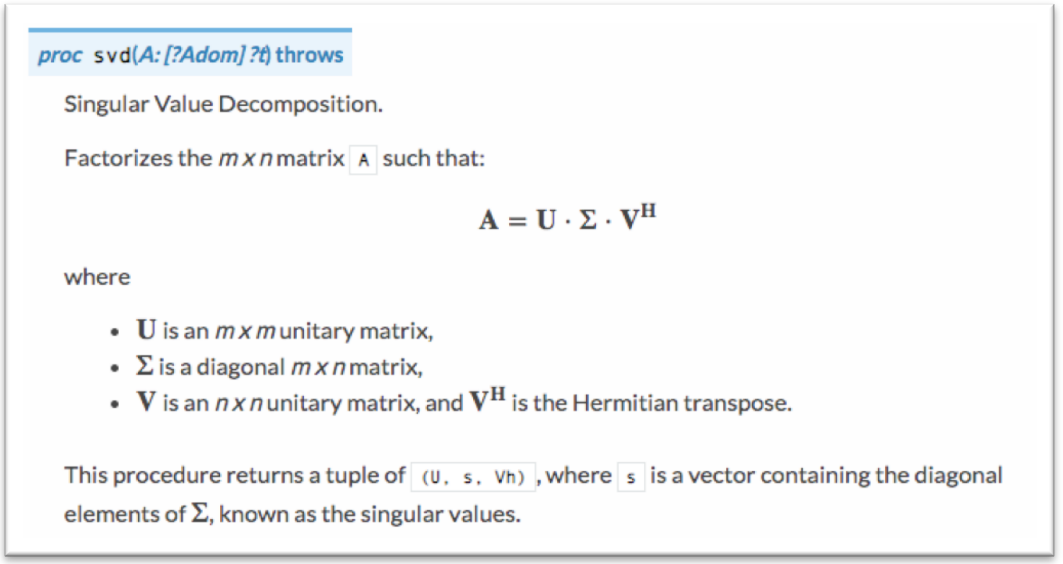
LinearAlgebra: This Effort

- **Improved feature set**
  - Added svd() procedure (singular value decomposition)
- **Improved usability**
  - BLAS and LAPACK dependencies only required if actually used
  - New BLAS and LAPACK flags allow for disabling dependencies
  - Shape preservation for promoted operations
- **Improved performance**
  - Optimized sparse matrix-matrix multiplication
  - Improved sparse matrix-matrix addition
    - Contributed by Kerim Tshimanga

LinearAlgebra: Impact - Features

- **Singular value decomposition now available**
  - Important procedure for many computations
    - e.g. PCA (principle component analysis)
  - Utilizes LAPACK

```
use LinearAlgebra;

var A = Matrix([3, 2, 2],
               [2, 3, -2],
               eltType=real);
var (U, s, Vh) = svd(A);
```



proc svd(*A: [?Adom] ?t*) throws

Singular Value Decomposition.

Factorizes the *m x n* matrix `A` such that:

$$\mathbf{A} = \mathbf{U} \cdot \Sigma \cdot \mathbf{V}^{\mathbf{H}}$$

where

- $\mathbf{U}$ is an *m x m* unitary matrix,
- Σ is a diagonal *m x n* matrix,
- $\mathbf{V}$ is an *n x n* unitary matrix, and $\mathbf{V}^{\mathbf{H}}$ is the Hermitian transpose.

This procedure returns a tuple of `(U, s, Vh)`, where `s` is a vector containing the diagonal elements of Σ, known as the singular values.

LinearAlgebra: Impact - Usability

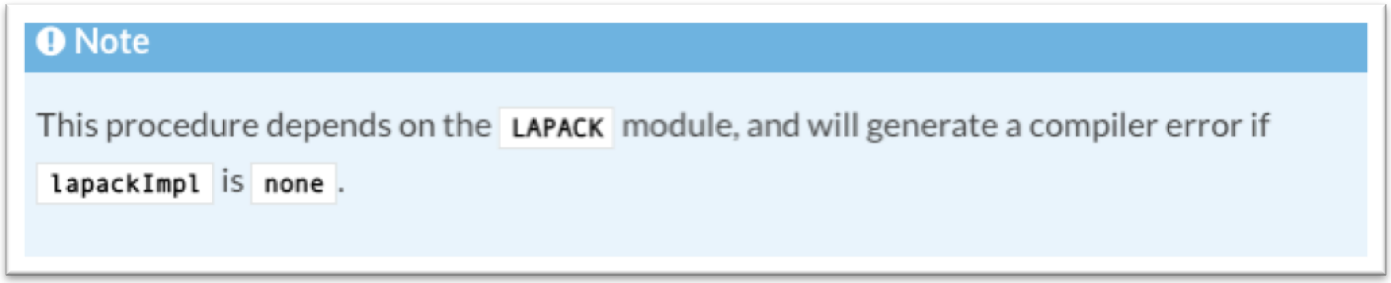
- **New config params in BLAS / LAPACK module:**
  - *blasImpl & lapackImpl*
    - Allows users to easily toggle BLAS/LAPACK implementations used
    - Sets header for common implementations (none, blas, mkl)

      ```
      chpl -s blasImpl=mkl -s lapackImpl=mkl
      ```

  - *blasHeader & lapackHeader*
    - Allows users to try previously untested BLAS/LAPACK implementations
    - Sets header explicitly for any implementation, overrides **Impl* flags

      ```
      chpl -s blasHeader=\"gsl_blas.h\"
      ```

- **Dependencies documented:**



LinearAlgebra: Impact - Usability

- **Dependencies only required when they are used:**

```
use LinearAlgebra;

// No usage of BLAS or LAPACK
var A = Matrix([0.0, 1.0, 1.0],
               [1.0, 0.0, 1.0],
               [1.0, 1.0, 0.0]);
var I = eye(3,3);
var B = A + I;
var A = Matrix(10, 4);

// 1.17: chpl –lblas –llapack example.chpl
// 1.18: chpl example.chpl
```

LinearAlgebra: Impact - Usability

- **Dependencies only required when they are used:**

```
use LinearAlgebra;

// eigvals() requires LAPACK
var A = Matrix([2.0, 1.0], [1.0, 2.0]);
var (eigenvalues, eigenvectors) = eigvals(A, right=true);
```

```
// 1.17: chpl –lblas –llapack example.chpl
// 1.18: chpl –llapack example.chpl
```

LinearAlgebra: Impact - Usability

- **Dependencies only required when they are used:**

```
use LinearAlgebra;

// mat-mat mult requires BLAS unless `–s BlasImpl=none` is set
var A = Matrix(3,5);
A = 2;
var AA = A.dot(A.T);
```

```
// 1.17 (BLAS):    chpl –lblas –llapack example.chpl
// 1.18 (BLAS):    chpl –lblas example.chpl
// 1.18 (native):    chpl –s blasImpl=none example.chpl
```

LinearAlgebra: Impact - Usability

- **Promoted operations now preserve shape**
  - Removed caveats about this in documentation
  - Element-wise operation methods not needed for dense matrices
    - Allows more natural usage of operations: +, -, *, /

```
// 1.17 element-wise operations
use LinearAlgebra;

var A = Matrix(3,3),
    B = Matrix(3,3);

var C = A.plus(B);
```

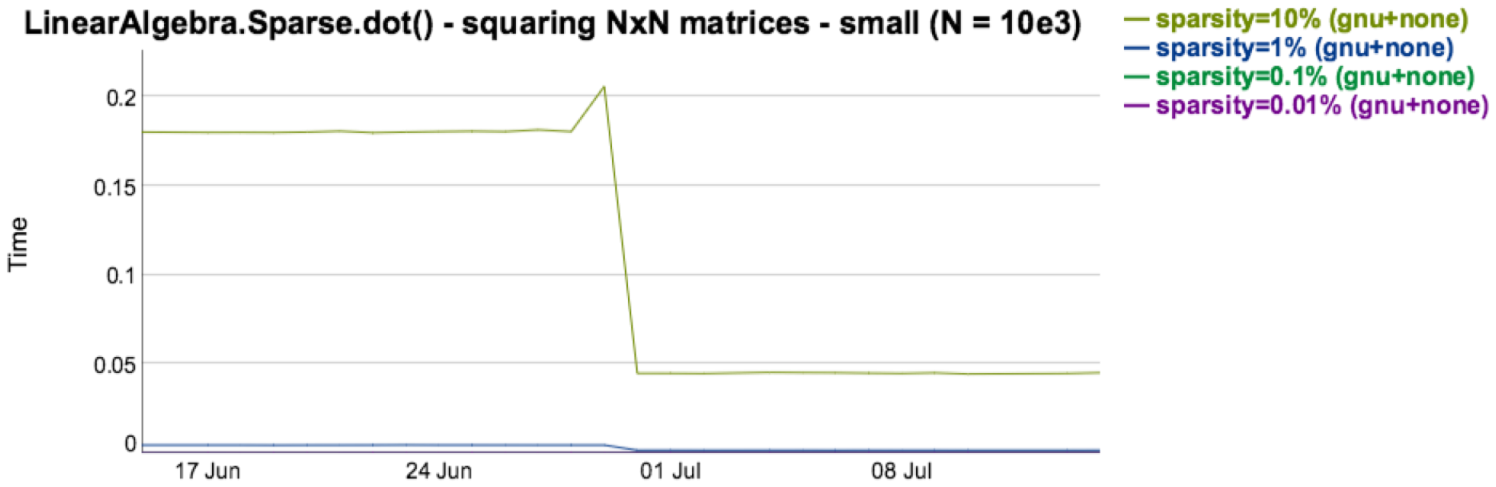
```
// 1.18 element-wise operations
use LinearAlgebra;

var A = Matrix(3,3),
    B = Matrix(3,3);

var C = A + B;
```

LinearAlgebra: Impact - Performance

- **Sparse matrix-matrix multiplication**
  - Switched sparse matrices to default to unsorted indices

    // Default array layout in LinearAlgebra.Sparse

    ```
    CS(compressedRows=true, sortedIndices=false)
    ```
  - Performance improvement scales with matrix density



LinearAlgebra: Next Steps

- **Distributed support**
  - Considering interfacing with ScaLAPACK
- **GPU support**
  - Considering interfacing cuBLAS or clBLAS
- **More features for dense and sparse modules**
- **More next steps tracked in issue #5753**

Crypto Package Module

Crypto

Background: Crypto package module uses OpenSSL

- Implemented with OpenSSL 1.0
- OpenSSL 1.1 has API changes and is in Ubuntu 18.04

This Effort: Support both OpenSSL 1.0 and 1.1 in Crypto

- Contributed by Sarthak Munshi

Impact: Crypto module more portable

Error-Handling in Standard Modules

Error-Handling: Background

- **Error handling recommended for use after 1.17**
  - However, we did not have much code that used error handling
    - made it difficult to build confidence in design and implementation
- **Want to avoid halts in standard modules**
  - Halts are hostile to users and prevent them from addressing errors
  - Halting acceptable only…
    …for unrecoverable problems
    …when performance penalty of error handling is too high
  - In particular, halting is currently considered acceptable for things like:
    - out-of-memory
    - bounds checking
    - cast checking
    - nil checking

Error-Handling: This Effort

- **Removed halts from remaining standard modules**
  - Converted “out error” pattern to error handling
  - Converted halts in several modules to error handling
    - DateTime, BigInteger, IO, Barrier, and a few others
  - Improved implementation in cases where halts were unnecessary
  - Downgraded some halts to warnings
    - calling start() on an already started timer
    - using `numTasks < 0` for dynamic iterators
- **Converted Mason to use error-handling**
- **Started on initial “users guide” for error-handling**
  - When to use error-handling and performance considerations
    - See #10703

Error-Handling: Impact and Next Steps

Impact:

- Improved quality of the standard modules
- Gained a bit more confidence in error-handling design/implementation
  - particularly from converting mason

Next Steps:

- Continue to put more weight on error-handling
- Remove halts from internal modules and distributions
- Formalize error-handling users guide

For More Information

For a more complete list of library changes in the 1.18 release, refer to the ‘Standard Modules / Library’, ‘Package Modules’ and ‘Bug Fixes’ sections in the **CHANGES.md** file.

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