

Package ‘MagmaQR’

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Type Package

Title Implementation of several matrix and linear algebra functions via the multi-GPU-based functionality in the MAGMA library

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Description Provides a client-server based interface to the 2 stage symmetric eigenvalue decomposition (`dsyevdx_2stage_m()`) multi-gpu/single-gpu routine from the MAGMA library. Can be used as replacement for the `eigen()` function in R for symmetric, double precision (the default in R) matrices. We get the server to check how many GPUs are present therefore we do not need CUDA/other interface to be present for compilation of the MagmaEigenNonsym package. required is the MAGMA library available (<http://icl.cs.utk.edu/magma/>) compiled as position independent code with a multi-threaded high performance LAPACK and -DMAGMA_ILP64 defined (an example `make.inc` file should be available in MAGMA download package).

NeedsCompilation yes

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LazyLoad yes

Depends R (>= 3.5), Rcpp (>= 0.11.0)

Imports Rcpp

LinkingTo Rcpp

SystemRequirements GNU make

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GetServerArgs	<i>Initialise shared memory on client and obtain server launch string.</i>
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Description

This function will create a CSharedMemory object that initialises the shared memory region and the semaphore used for comms between client and server. If the object is already initialised it is removed and reinitialised. Returns a string of the form "-n 10000 -v 1 -g 3 -m /syevx_<PID_of_client> -s /sem_<PID_of_client> -p" that can be used to launch a qr_server process that will accept matrix data on which to perform QR factorisation and return the QR matrix.

Usage

```
GetServerArgs(matrixDimension, withVectors, numGPUsWanted, memName, semName,
              printDetails)
```

Arguments

matrixDimension	- type (integer) - the dimension of the (assumed square) matrix
withVectors	- type (boolean) - this is always set to true. It is a legacy parameter from Joshs Eigendecomposition code.
numGPUsWanted	- type (string) - The number of GPUs to use
memName	- type (string) - a name to give to the named shared memory region (will be created in /dev/shm/) and defaults to the user name if nothing specified
semName	- type (string) - a name to give to the semaphore (will be placed in /dev/shm) and defaults to the user name if nothing specified
printDetails	- type (integer 0 1 2) - 0 = don't print, 1 = print details of server progress to screen; 2 = print to log (not functional)

Value

- type (string) A string that can be used a command line arguments to run the qr_server executable

MagmaQR	<i>MagmaQR - provides a fast replacement for the qr() function, using GPU based MAGMA library routine.</i>
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Description

Implements the symmetric eigenvalue decomposition using the MAGMA library (<http://icl.cs.utk.edu/magma/index.html>) 2-stage multi-GPU implementation with 64 bit integer interface. Currently only for real symmetric matrices. In this case it provides a direct replacement for R function `eigen(symmetric=T)` and also provides an efficient function for producing the square root and inverse square root of the input matrix. The package uses the 64 bit integer MAGMA library by a client-server shared memory architecture. This removes the problem that can arise with larger datasets where R only provides the 32 bit BLAS/LAPACK interface. The server side code checks how many GPUs are present so the client side R package code does not require CUDA/other interface to be present. The server

side code requires the MAGMA library to be available (<http://icl.cs.utk.edu/magma/>) compiled as position independent code (shared library) with a multi-threaded high performance LAPACK and -DMAGMA_ILP64 defined (an example make.inc file should be available in MAGMA download package). The server code also requires an OpenCL library to be installed which is used to get the number of GPUs present on a system. This package can be used in conjunction with HiPLARb and HiPLARM that require high performance, but single-threaded BLAS routines, which will then degrade the performance of some routines (such as `eigen()` and possibly `svd()`) which require a multi threaded BLAS to operate effectively.

Compilation of the R package the 'client side' code: Optionally set `MAGMA_HOME` and `CUDA_ROOT` as per the server side instructions. This will allow the client to compile the server code during package install. Setting the OpenCL platform string and device type:

Compilation of the 'server side' code: Requires environment variables `MAGMA_HOME` to be set to where the MAGMA install is present. `MAGMA_HOME=/usr/local/magma` is the default. The CUDA version of MAGMA requires `CUDA_ROOT` to be set `CUDA_ROOT=/usr/local/cuda` is the default. The server code uses OpenCL to determine how many GPUs are present on the system it is being run on. The default platform string is stored in a file in `<R library path>/rcppMagamSYEVD/extdata/platformstring` and contains the default platform string "NVidia", and the default device is set to "GPU". See the `platformstring.txt` file for other options. If these libraries and variables are set correctly then the server side code will be compiled automatically when the package is installed. If failing installation on install then whenever the package is loaded into the R environment using `library(MagmaQR)` the system will attempt to compile the server code.

N.B. Calling the `solve_mgpu()` function with argument `overwrite=TRUE` will cause an *overwrite of the input matrix data* with the eigenvectors of the original matrix data (if they are requested). This is done to potentially reduce the memory footprint of the function. If `overwrite=TRUE` then please ensure the original matrix is copied if the data needs to be used after the function is called. Using `overwrite=FALSE` will return the usual list of results in `$vectors` and `$values` list items of the result object.

Details

Package:	MagmaQR
Type:	Package
Version:	1.0.0
Date:	2016-02-01
License:	GPL-3 + file LICENCE
LazyLoad:	yes

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References

Stanimire Tomov, Jack Dongarra, Marc Baboulin, Towards dense linear algebra for hybrid GPU accelerated manycore systems, *Parallel Computing*, Volume 36, Issues 5-6, June 2010, Pages 232-240, ISSN 0167-8191, <http://dx.doi.org/10.1016/j.parco.2009.12.005>.

@article title = Towards dense linear algebra for hybrid GPU accelerated manycore systems, author = Stanimire Tomov and Jack Dongarra and Marc Baboulin, booktitle = Parallel Matrix Algorithms and Applications, doi = 10.1016/j.parco.2009.12.005, issn = 0167-8191, journal = Parallel Computing, month = jun, number = 5-6, pages = 232–240, posted-at = 2010-12-17 09:48:58, priority = 2, volume = 36, year = 2010

Solca, Raffaele; Haidar, Azzam; Tomov, Stanimire; Schulthess, Thomas C.; Dongarra, Jack, "Abstract: A Novel Hybrid CPU-GPU Generalized Eigensolver for Electronic Structure Calculations Based on Fine Grained Memory Aware Tasks," in High Performance Computing, Networking, Storage and Analysis (SCC), 2012 SC Companion: , vol., no., pp.1338-1339, 10-16 Nov. 2012 doi: 10.1109/SC.Companion.2012.173

@articleHaidar:2014:NHC:2747699.2747703, author = Haidar, Azzam and Tomov, Stanimire and Dongarra, Jack and Solca, Raffaele and Schulthess, Thomas, title = A Novel Hybrid CPU-GPU Generalized Eigensolver for Electronic Structure Calculations Based on Fine-grained Memory Aware Tasks, journal = Int. J. High Perform. Comput. Appl., issue_date = May 2014, volume = 28, number = 2, month = may, year = 2014, issn = 1094-3420, pages = 196–209, numpages = 14, url = <http://dx.doi.org/10.1177/1094342013502097>, doi = 10.1177/1094342013502097, acmid = 2747703, publisher = Sage Publications, Inc., address = Thousand Oaks, CA, USA, keywords = Eigensolver, GPU, electronic structure calculations, generalized eigensolver, high performance, hybrid, multicore, two-stage,

See Also

eigen

Examples

```
# setup

# setup
set.seed(101)
n <- 10000
ngpu <- 4
K <- matrix(sample(c(0,1), n*n, TRUE ), nrow=n)
res <- tcrossprod(K)
print(res[1:5,1:5])

# CPU based
library(MagmaQR)
MagmaQR::RunServer( matrixMaxDimension=n, numGPUsWanted=ngpu, memName="/syevd_mem", semName="/syevd_sem",

qGPU <- MagmaQR::qr_mgpu(res)

## CPU
qCPU <- qr.Q(qr(res))

print(qGPU[1:5, 1:5])
print("-----")
print(qCPU[1:5, 1:5])

print(c("Test Sum = ", sum(qGPU - qCPU) ))

StopServer() # Client signals to server to terminate
```

MakeServer	<i>Creates the server executable.</i>
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Description

Creates syevd_server executable using a call to 'make' and the makefile and make.inc information present in the <package root>/src directory. Users have to set the following variable in make.inc :
MAGMALIB=\$(MAGMA_HOME)/lib # The path to the MAGMA library

Users must ensure that MAGMA_HOME and possibly CUDA_ROOT environment variables have been set in the shells environment or the variables can be set using environmentSetup paramater. e.g.
"environmentSetup="env MAGMA_HOME=/data/bow355/A_275ERCP_R_MAGMA/magma-1.7.0
CUDA_ROOT=/cm/shared/apps/cuda65/toolkit/6.5.14 "

Usage

```
MakeServer(environmentSetup = "", target = "all")
```

Arguments

environmentSetup	- type (string) e.g. "env LD_LIBRARY_PATH=/usr/local/magma-1.7.1:\$LD_LIBRARY_PATH"
target	- type (string) The make target e.g. all clean dist-clean install

Value

A character vector containing output of the make process

qr_mgpu	<i>Function used to obtain the eigenvalue decomposition (EVD) of a non-symmetric matrix using a MAGMA 2-stage multi-gpu EVD algorithm</i>
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Description

This function performs the eigenvalue decomposition of the input matrix and returns the eigenvalues and (if requested) the eigenvectors of the input matrix in the returned list, identical to the base R eigen() function. If overwrite=TRUE then the eigenvectors are copied into the ***input matrix*** and the original matrix data is overwritten. The method involves the offload of the matrix data to a separate syevd_server executable by copying data into a shared memory area and signalling to the server that the data is available. This function will block until the server has completed the decomposition. The function checks that the input is square, however it does not check that the matrix is symmetric. N.B. The maximum size allowed of the input matrix is goverend by what was provided in the MagmaQR::RunServer() function. The server will automatically be restarted with a larger shared memory area if user wants to perorm EVD on a larger matrix.

Usage

```
qr_mgpu(matrix)
```

Arguments

matrix - the input matrix to be used in eigenvalue decomposition. It is assumed to be square

Value

A list that contains the eigenvalues and if requested the eigenvectors. If `overwrite==TRUE` then the eigenvectors are copied into the `***input matrix***`

RunServer	<i>Creates the R client side shared memory region and then launches a server process which is given access to the shared region. The server then waits for the R client to give it a matrix on which it will compute the eigenvalue decomposition of using a syevdx_2stage MAGMA library function.</i>
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Description

Creates the R client side shared memory region and then launches a server process which is given access to the shared region. The server then waits for the R client to give it a matrix on which it will compute the eigenvalue decomposition of using a syevdx_2stage MAGMA library function.

Usage

```
RunServer(environmentSetup = "", numGPUsWanted = 0,
          matrixMaxDimension = 0, memName = "", semName = "", print = 0)
```

Arguments

environmentSetup - type (string) - Environment variables that need to be set, such as library include paths

numGPUsWanted - type (string) - The number of GPUs to use in for the symmetric eigenvalue (syevd) computation

matrixMaxDimension - type (integer) - The maximum matrix size that this server instance can handle
- sets the shared memory size

memName - type (string) - A name to give to the named shared memory region (will be created in /dev/shm/) and defaults to the user name if nothing specified

semName - type (string) - A name to give to the semaphore (will be placed in /dev/shm) and defaults to the user name if nothing specified

print - type (integer 0|1|2) - 0 = don't print, 1 = print details of server progress to screen; 2 = print to log (not functional)

Details

This function creates a command line with which to call the syevd_server executable and then calls the executable with a non-blocking system() call to launch the server process. The server then waits for the client to send it matrix data via the syevdx_client() function. The matrixMaxDimension paramater specifies the largest size matrix that can be processed by this instance of the syevd_server().

Value

a vector character values containing output of the make process

StopServer	<i>Function signals to the server through shared memory region to terminate from its main loop and then deletes the client CSharedMemory object</i>
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Description

Function signals to the server through shared memory region to terminate from its main loop and then deletes the client CSharedMemory object

Usage

StopServer()

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MAGMA, eigen, GPU, EVD

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