S05: High Performance Computing with CUDA

CUDA Libraries

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Outline

- CUDA libraries:
  - CUBLAS: BLAS implementation
  - CUFFT: FFT implementation
- Using CUFFT to solve a Poisson equation with spectral methods:
  - How to use the profile
  - Optimization steps
- Accelerating MATLAB code with CUDA

CUBLAS

CUBLAS is an implementation of BLAS (Basic Linear Algebra Subprograms) on top of the CUDA driver. It allows access to the computational resources of NVIDIA GPUs.

The library is self-contained at the API level, that is, no direct interaction with the CUDA driver is necessary.

The basic model by which applications use the CUBLAS library is to:

- **create matrix and vector objects in GPU memory space,**
- **fill them with data,**
- **call a sequence of CUBLAS functions,**
- **upload the results from GPU memory space back to the host.**

CUBLAS provides helper functions for creating and destroying objects in GPU space, and for writing data to and retrieving data from these objects.

Supported features

- **BLAS functions implemented (single precision only):**
  - **Real data: level 1, 2 and 3**
  - **Complex data: level1 and CGEMM**

(Level 1=vector vector O(N), Level 2= matrix vector O(N^2), Level 3=matrix matrix O(N^3))

- **For maximum compatibility with existing Fortran environments, CUBLAS uses column-major storage, and 1-based indexing:**

Since C and C++ use row-major storage, this means applications cannot use the native C array semantics for two-dimensional arrays. Instead, macros or inline functions should be defined to implement matrices on top of one-dimensional arrays.

Using CUBLAS

•The interface to the CUBLAS library is the header file cublas.h

•Function names: cublas(Original name).
cublasSgemm

•Because the CUBLAS core functions (as opposed to the helper functions) do not return error status directly, CUBLAS provides a separate function to retrieve the last error that was recorded, to aid in debugging

•CUBLAS is implemented using the C-based CUDA tool chain, and thus provides a C-style API. This makes interfacing to applications written in C or C++ trivial.

cublasInit, cublasShutdown

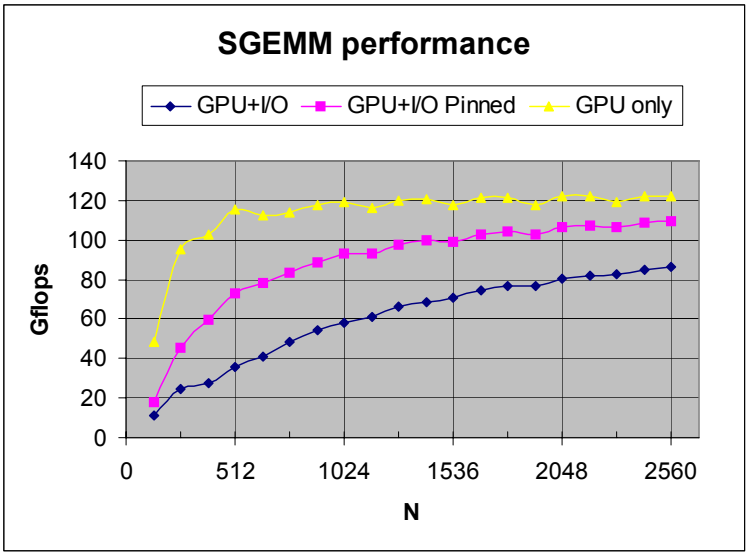
cublasStatus cublasInit()

initializes the CUBLAS library and must be called before any other CUBLAS API function is invoked. It allocates hardware resources necessary for accessing the GPU.

cublasStatus cublasShutdown()

releases CPU-side resources used by the CUBLAS library. The release of GPU-side resources may be deferred until the application shuts down.

CUBLAS performance



cublasGetError, cublasAlloc, cublasFree

cublasStatus cublasGetError()

returns the last error that occurred on invocation of any of the CUBLAS core functions. While the CUBLAS helper functions return status directly, the CUBLAS core functions do not, improving compatibility with those existing environments that do not expect BLAS functions to return status. Reading the error status via cublasGetError() resets the internal error state to CUBLAS_STATUS_SUCCESS..

cublasStatus cublasAlloc (**int n, int elemSize, void **devicePtr**)

creates an object in GPU memory space capable of holding an array of n elements, where each element requires elemSize bytes of storage.
Note that this is a device pointer that cannot be dereferenced in host code.
cublasAlloc() is a wrapper around cudaMalloc().
Device pointers returned by cublasAlloc() can therefore be passed to any CUDA device kernels, not just CUBLAS functions.

cublasStatus cublasFree(const void *devicePtr)

destroys the object in GPU memory space referenced by devicePtr.

cublasSetVector, cublasGetVector

cublasStatus cublasSetVector(int n, int elemSize, const void *x, int incx, void *y, int incy)

copies n elements from a vector x in CPU memory space to a vector y in GPU memory space. Elements in both vectors are assumed to have a size of elemSize bytes. Storage spacing between consecutive elements is incx for the source vector x and incy for the destination vector y

cublasStatus cublasGetVector(int n, int elemSize, const void *x, int incx, void *y, int incy)

copies n elements from a vector x in GPU memory space to a vector y in CPU memory space. Elements in both vectors are assumed to have a size of elemSize bytes. Storage spacing between consecutive elements is incx for the source vector x and incy for the destination vector y

cublasSetMatrix, cublasGetMatrix

cublasStatus cublasSetMatrix(int rows, int cols, int elemSize, const void *A, int lda, void *B, int ldb)

copies a tile of rows x cols elements from a matrix A in CPU memory space to a matrix B in GPU memory space. Each element requires storage of elemSize bytes. Both matrices are assumed to be stored in column-major format, with the leading dimension (that is, the number of rows) of source matrix A provided in lda, and the leading dimension of destination matrix B provided in ldb.

cublasStatus cublasGetMatrix(int rows, int cols, int elemSize, const void *A, int lda, void *B, int ldb)

copies a tile of rows x cols elements from a matrix A in GPU memory space to a matrix B in CPU memory space. Each element requires storage of elemSize bytes. Both matrices are assumed to be stored in column-major format, with the leading dimension (that is, the number of rows) of source matrix A provided in lda, and the leading dimension of destination matrix B provided in ldb.

Calling CUBLAS from FORTRAN

Fortran-to-C calling conventions are not standardized and differ by platform and toolchain.

In particular, differences may exist in the following areas:

- **symbol names (capitalization, name decoration)**
- **argument passing (by value or reference)**
- **passing of string arguments (length information)**
- **passing of pointer arguments (size of the pointer)**
- **returning floating-point or compound data types (for example, single-precision or complex data type)**

•CUBLAS provides wrapper functions (in the file fortran.c) that need to be compiled with the user preferred toolchain. Providing source code allows users to make any changes necessary for a particular platform and toolchain.

Calling CUBLAS from FORTRAN

Two different interfaces:

•**Thunking** (define CUBLAS_USE_THUNKING when compiling fortran.c): allow interfacing to existing Fortran applications without any changes to the application. During each call, the wrappers allocate GPU memory, copy source data from CPU memory space to GPU memory space, call CUBLAS, and finally copy back the results to CPU memory space and deallocate the GPGPU memory. As this process causes significant call overhead, these wrappers are intended for light testing,not for production code.

•**Non-Thunking** (default):
intended for production code, substitute device pointers for vector and matrix arguments in all BLAS functions. To use these interfaces, existing applications need to be modified slightly to allocate and deallocate data structures in GPGPU memory space (using CUBLAS_ALLOC and CUBLAS_FREE) and to copy data between GPU and CPU memory spaces (using CUBLAS_SET_VECTOR, CUBLAS_GET_VECTOR, CUBLAS_SET_MATRIX, and CUBLAS_GET_MATRIX).

FORTRAN 77 Code example:

```
program matrixmod
implicit none
integer M, N
parameter (M=6, N=5)
real*4 a(M,N)
integer i, j

do j = 1, N
  do i = 1, M
     a(i,j) = (i-1) * M + j
  enddo
enddo

call modify (a, M, N, 2, 3, 16.0, 12.0)

do j = 1, N
  do i = 1, M
     write(*,"(F7.0$)") a(i,j)
  enddo
  write (*,*) ""
enddo

stop
end
```

```
subroutine modify (m, ldm, n, p, q, alpha, beta)
implicit none
integer ldm, n, p, q
real*4 m(ldm,*), alpha, beta

external sscal

call sscal (n-p+1, alpha, m(p,q), ldm)

call sscal (ldm-p+1, beta, m(p,q), 1)

return
end
```


FORTRAN 77 Code example: Non-thunking interface

```
program matrixmod
implicit none
integer M, N, sizeof_real, devPtrA
parameter (M=6, N=5, sizeof_real=4)
real*4 a(M,N)
integer i, j, stat
external cublas_init, cublas_set_matrix,cublas_get_matrix
external cublas_shutdown, cublas_alloc
integer cublas_alloc

do j = 1, N
  do i = 1, M
     a(i,j) = (i-1) * M + j
  enddo
enddo

call cublas_init
stat = cublas_alloc(M*N, sizeof_real, devPtrA)
if (stat .NE. 0) then
   write(*,*) "device memory allocation failed"
   stop
endif

call cublas_set_matrix (M, N, sizeof_real, a, M, devPtrA, M)
call modify (devPtrA, M, N, 2, 3, 16.0, 12.0)
call cublas_get_matrix (M, N, sizeof_real, devPtrA, M, a, M)
call cublas_free(devPtrA)
call cublas_shutdown
```

```
do j = 1, N
  do i = 1, M
     write(*,"(F7.0$)") a(i,j)
  enddo
  write (*,*) ""
enddo

stop
end

#define IDX2F(i,j,ld) ((((j)-1)*(ld))+((i)-1)

subroutine modify (devPtrM, ldm, n, p, q, alpha, beta)
implicit none
integer ldm, n, p, q
integer sizeof_real, devPtrM
parameter (sizeof_real=4)
real*4  alpha, beta
call cublas_sscal (n-p+1, alpha,
                   devPtrM+IDX2F(p,q,ldm)*sizeof_real,
                   ldm)
call cublas_sscal (ldm-p+1, beta,
                   devPtrM+IDX2F(p,q,ldm)*sizeof_real,
                   1)
return
end
```

If using fixed format check that the line length is below the 72 column limit !!!

CUFFT

The Fast Fourier Transform (FFT) is a divide-and-conquer algorithm for efficiently computing discrete Fourier transform of complex or real-valued data sets.

The FFT is one of the most important and widely used numerical algorithms.

CUFFT, the "CUDA" FFT library, provides a simple interface for computing parallel FFT on an NVIDIA GPU. This allows users to leverage the floating-point power and parallelism of the GPU without having to develop a custom, GPU-based FFT implementation.

Supported features

- 1D, 2D and 3D transforms of complex and real-valued data
- Batched execution for doing multiple 1D transforms in parallel
- 1D transform size up to 8M elements
- 2D and 3D transform sizes in the range [2,16384]
- In-place and out-of-place transforms for real and complex data.

CUFFT Types and Definitions

type cufftHandle:
is a handle type used to store and access CUFFT plans

type cufftResults:
is an enumeration of values used as API function values return values.

CUFFT_SUCCESS	Any CUFFT operation is successful.
CUFFT_INVALID_PLAN	CUFFT is passed an invalid plan handle.
CUFFT_ALLOC_FAILED	CUFFT failed to allocate GPU memory.
CUFFT_INVALID_TYPE	The user requests an unsupported type.
CUFFT_INVALID_VALUE	The user specifies a bad memory pointer.
CUFFT_INTERNAL_ERROR	Used for all internal driver errors.
CUFFT_EXEC_FAILED	CUFFT failed to execute an FFT on the GPU.
CUFFT_SETUP_FAILED	The CUFFT library failed to initialize.
CUFFT_SHUTDOWN_FAILED	The CUFFT library failed to shut down.
CUFFT_INVALID_SIZE	The user specifies an unsupported FFT size.

Transform types

- **The library supports complex and real data transforms:**
  CUFFT_C2C, CUFFT_C2R ,CUFFT_R2C
  with directions:
  CUFFT_FORWARD (-1) and CUFFT_BACKWARD (1)
  according to the sign of the complex exponential term
- **For complex FFTs, the input and output arrays must interleaved the real and imaginary part (cufftComplex type is defined for this purpose)**
- **For real-to-complex FFTs, the output array holds only the non-redundant complex coefficients:**
  N -> N/2+1
  N0 x N1 x …. x Nn -> N0 x N1 x …. X (Nn/2+1)
  To perform in-place transform the input/output needs to be padded

More on transforms

- **For 2D and 3D transforms, CUFFT performs transforms in row-major (C-order).**
- **If calling from FORTRAN or MATLAB, remember to change the order of size parameters during plan creation.**
- **CUFFT performs un-normalized transforms:**

  IFFT(FFT(A))= length(A)*A
- **CUFFT API is modeled after FFTW. Based on plans, that completely specify the optimal configuration to execute a particular size of FFT.**
- **Once a plan is created, the library stores whatever state is needed to execute the plan multiple times without recomputing the configuration: it works very well for CUFFT, because different kinds of FFTs require different thread configurations and GPU resources.**

cufftPlan1d()

cufftResult cufftPlan1d(cufftHandle *plan, int nx, cufftType type, int batch);

creates a 1D FFT plan configuration for a specified signal size and data type.
The batch input parameter tells CUFFT how many 1D transforms to configure.

Input:

plan	Pointer to a cufftHandle object
nx	The transform size (e.g., 256 for a 256-point FFT)
type	The transform data type (e.g., CUFFT_C2C for complex-to-complex)
batch	Number of transforms of size nx

Output:

plan	Contains a CUFFT 1D plan handle value

cufftPlan2d()

cufftResult cufftPlan2d(cufftHandle *plan, int nx, int ny, cufftType type);

creates a 2D FFT plan configuration for a specified signal size and data type.

Input:

- plan Pointer to a cufftHandle object
- nx The transform size in X dimension
- ny The transform size in Y dimension
- type The transform data type (e.g., CUFFT_C2C for complex-to-complex)

Output:

- plan Contains a CUFFT 2D plan handle value

cufftPlan3d()

cufftResult cufftPlan3d(cufftHandle *plan, int nx, int ny, int nz, cufftType type);

creates a 3D FFT plan configuration for a specified signal size and data type.

Input:

- plan Pointer to a cufftHandle object
- nx The transform size in X dimension
- ny The transform size in Y dimension
- nz The transform size in Z dimension
- type The transform data type (e.g., CUFFT_C2C for complex-to-complex)

Output:

- plan Contains a CUFFT 3D plan handle value

cufftDestroy(),

cufftResult cufftDestroy(cufftHandle plan);

frees all GPU resources associated with a CUFFT plan and destroys the internal plan data structure. This function should be called once a plan is no longer needed to avoid wasting GPU memory**.**

Input:

plan cufftHandle object

cufftExecC2C()

cufftResult cufftExecC2C(cufftHandle plan,
cufftComplex *idata, cufftComplex *odata,
int direction);

executes a CUFFT complex to complex transform plan.CUFFT uses as input data the GPU memory pointed to by the idata parameter. This function stores the Fourier coefficients in the odata array. If idata and odata are the same, this method does an in-place transform.

Input:

plan	cufftHandle object for the plane to update
idata	Pointer to the input data (in GPU memory) to transform
odata	Pointer to the output data (in GPU memory)
direction	The transform direction (CUFFT_FORWARD or CUFFT_BACKWARD)

Output:

odata	Contains the complex Fourier coefficients)

cufftExecR2C()

cufftResult cufftExecR2C(cufftHandle plan,
cufftReal *idata, cufftComplex *odata);

executes a CUFFT real to complex transform plan.CUFFT uses as input data the GPU memory pointed to by the idata parameter. This function stores the Fourier coefficients in the odata array. If idata and odata are the same, this method does an in-place transform.
The output hold only the non-redundant complex Fourier coefficients.

Input:

plan	Pointer to a cufftHandle object
idata	Pointer to the input data (in GPU memory) to transform
odata	Pointer to the output data (in GPU memory)

Output:

odata	Contains the complex Fourier coefficients

cufftExecC2R()

cufftResult cufftExecC2R(cufftHandle plan,
cufftComplex *idata, cufftReal *odata);

executes a CUFFT complex to real transform plan. CUFFT uses as input data the GPU memory pointed to by the idata parameter. This function stores the Fourier coefficients in the odata array. If idata and odata are the same, this method does an in-place transform.
The input hold only the non-redundant complex Fourier coefficients.

Input:

plan	Pointer to a cufftHandle object
idata	Pointer to the complex input data (in GPU memory) to transform
odata	Pointer to the real output data (in GPU memory)

Output:
odata Contains the real-valued Fourier coefficients

Accuracy and performance

The CUFFT library implements several FFT algorithms, each with different performances and accuracy.

The best performance paths correspond to transform sizes that:

1. **Fit in CUDA'a shared memory**
2. **Are powers of a single factor (e.g. power-of-two)**

If only condition 1 is satisfied, CUFFT uses a more general mixed-radix factor algorithm that is slower and less accurate numerically.

If none of the above conditions is satisfied, CUFFT uses an out-of-place, mixed-radix algorithm that stores all intermediate results in global GPU memory.

One notable exception is for long 1D transforms, where CUFFT uses a distributed algorithm that perform 1D FFT using 2D FFT, where the dimensions of the 2D transform are factors of

CUFFT does not implement any specialized algorithms for real data, and so there is no direct performance benefit to using real to complex (or complex to real) plans instead of complex to complex. For this release, the real data API exists primarily for convenience

Code example: 1D complex to complex transforms

```
#define NX 256
#define BATCH 10

cufftHandle plan;
cufftComplex *data;
cudaMalloc((void**)&data, sizeof(cufftComplex)*NX*BATCH);

/* Create a 1D FFT plan. */
 cufftPlan1d(&plan, NX, CUFFT_C2C, BATCH);

 /* Use the CUFFT plan to transform the signal in place. */
 cufftExecC2C(plan, data, data, CUFFT_FORWARD);

/* Inverse transform the signal in place. */
 cufftExecC2C(plan, data, data, CUFFT_INVERSE);

/* Note:
   (1) Divide by number of elements in data-set to get back original data
   (2) Identical pointers to input and output arrays implies in-place transformation
 */

 /* Destroy the CUFFT plan. */
   cufftDestroy(plan);

   cudaFree(data);
```


Code example:
2D complex to complex transform

```
#define NX 256
#define NY 128

cufftHandle plan;
cufftComplex *idata, *odata;
cudaMalloc((void**)&idata, sizeof(cufftComplex)*NX*NY);
cudaMalloc((void**)&odata, sizeof(cufftComplex)*NX*NY);

/* Create a 1D FFT plan. */
 cufftPlan2d(&plan, NX,NY, CUFFT_C2C);

 /* Use the CUFFT plan to transform the signal out of place. */
 cufftExecC2C(plan, idata, odata, CUFFT_FORWARD);

/* Inverse transform the signal in place. */
 cufftExecC2C(plan, odata, odata, CUFFT_INVERSE);

/* Note:
    Different pointers to input and output arrays implies out of place transformation
 */

 /* Destroy the CUFFT plan. */
  cufftDestroy(plan);

   cudaFree(idata), cudaFree(odata);
```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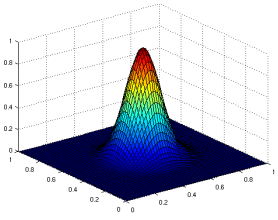
CUDA Example

Fourier-spectral Poisson Solver

Overview

In this example, we want to solve a Poisson equation on a rectangular domain with periodic boundary conditions using a Fourier-spectral method.



This example will show how to use the FFT library, transfer the data to/from GPU and perform simple computations on the GPU.

Mathematical background

$$\nabla^2 \phi = r \xrightarrow{FFT} -(k_x^2 + k_y^2)\hat{\phi} = \hat{r}$$

1. Apply 2D forward FFT to r to obtain r(k), where k is the wave number
2. Apply the inverse of the Laplace operator to r(k) to obtain u(k): simple element-wise division in Fourier space

$$\hat{\phi} = -\frac{\hat{r}}{(k_x^2 + k_y^2)}$$

3. Apply 2D inverse FFT to u(k) to obtain u

Reference MATLAB implementation

```
% No. of Fourier modes
      N = 64;
% Domain size (assumed square)
      L = 1;
% Characteristic width of f (make << 1)
      sig = 0.1;
% Vector of wavenumbers
      k = (2*pi/L)*[0:(N/2-1) (-N/2):(-1)];
%Matrix of (x,y) wavenumbers corresponding
% to Fourier mode (m,n)
      [KX KY]  = meshgrid(k,k);
% Laplacian matrix acting on the wavenumbers
      delsq = -(KX.^2 + KY.^2);
% Kludge to avoid division by zero for
% wavenumber (0,0).
% (this waveno. of fhat  should be zero anyway!)
      delsq(1,1) = 1;
% Grid spacing
      h = L/N;
      x = (0:(N-1))*h ;
      y = (0:(N-1))*h;
      [X Y] = meshgrid(x,y);
```

```
% Construct RHS f(x,y) at the Fourier gridpoints
      rsq = (X-0.5*L).^2 + (Y-0.5*L).^2;
      sigsq = sig^2;
      f = exp(-rsq/(2*sigsq)).*…
          (rsq - 2*sigsq)/(sigsq^2);
% Spectral inversion of Laplacian
      fhat = fft2(f);
      u = real(ifft2(fhat./delsq));
% Specify arbitrary constant by forcing corner
%  u = 0.
      u = u - u(1,1);
%  Compute L2 and Linf norm of error
      uex = exp(-rsq/(2*sigsq));
      errmax = norm(u(:)-uex(:),inf);
      errmax2 = norm(u(:)-uex(:),2)/(N*N);
%  Print L2 and Linf norm of error
      fprintf('N=%d\n',N);
      fprintf('Solution at (%d,%d): ',N/2,N/2);
      fprintf('computed=%10.6f …
          reference = %10.6f\n',u(N/2,N/2),
      uex(N/2,N/2));
       fprintf('Linf err=%10.6e L2 norm
            err = %10.6e\n',errmax, errmax2);
```

http://www.atmos.washington.edu/2005Q2/581/matlab/pois_FFT.m

Implementation steps

The following steps need to be performed:

1. Allocate memory on host: r (NxN), u (NxN) , kx (N) and ky (N)
2. Allocate memory on device: r_d, u_d, kx_d, ky_d
3. Transfer r, kx and ky from host memory to the correspondent arrays on device memory
4. Initialize plan for FFT
5. Compute execution configuration
6. Transform real input to complex input
7. 2D forward FFT
8. Solve Poisson equation in Fourier space
9. 2D inverse FFT
10. Transform complex output to real input and apply scaling
11. Transfer results from the GPU back to the host

We are not taking advantage of the symmetries (C2C transform for real data) to keep the code simple.

Solution walk-through (steps 1-2)

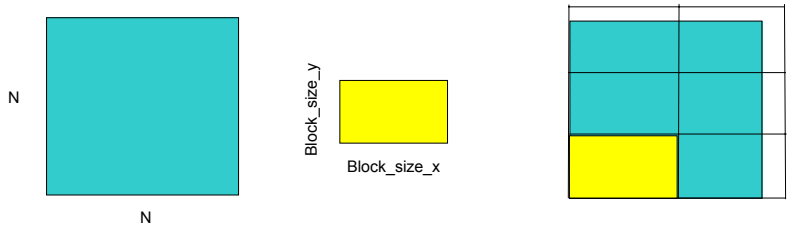
```
/*Allocate arrays on the host */
      float *kx, *ky, *r;
      kx = (float *) malloc(sizeof(float*N);
      ky = (float *) malloc(sizeof(float*N);
      r   = (float *) malloc(sizeof(float*N*N);

/* Allocate array on the GPU with cudaMalloc */
      float *kx_d, *ky_d, *r_d;
      cudaMalloc( (void **) &kx_d, sizeof(cufftComplex)*N);
      cudaMalloc( (void **) &ky_d, sizeof(cufftComplex)*N);
      cudaMalloc( (void **) &r_d  , sizeof(cufftComplex)*N*N);

      cufftComplex *r_complex_d;
      cudaMalloc( (void **) &r_complex_d, sizeof(cufftComplex)*N*N);
```


Code walk-through (steps 3-4)

```
/* Initialize r, kx and ky on the host */
  ……
/*Transfer data from host to device with
  cudaMemcpy(target, source, size, direction)*/
 cudaMemcpy (kx_d, kx, sizeof(float)*N    , cudaMemcpyHostToDevice);
 cudaMemcpy (ky_d, ky, sizeof(float)*N    , cudaMemcpyHostToDevice);
 cudaMemcpy (r_d  , r   , sizeof(float)*N*N, cudaMemcpyHostToDevice);

/* Create plan for CUDA FFT (interface similar to FFTW) */
  cufftHandle plan;
  cufftPlan2d( &plan, N, N, CUFFT_C2C);
```


Code walk-through (step 5)

```
/* Compute the execution configuration
   NB: block_size_x*block_size_y = number of threads
       On G80  number of threads < 512  */
  dim3 dimBlock(block_size_x, block_size_y);
  dim3 dimGrid (N/dimBlock.x, N/dimBlock.y);

/* Handle N not multiple of block_size_x or block_size_y */
  if (N % block_size_x  !=0 ) dimGrid.x+=1;
  if (N % block_size_y  !=0 ) dimGrid.y+=1
```



Code walk-through (step 6-10)

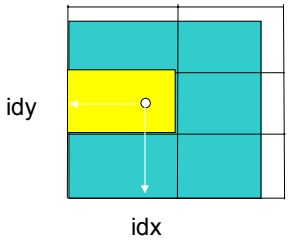
```
/* Transform real input to complex input */
  real2complex<<<dimGrid, dimBlock>>> (r_d, r_complex_d, N);

/* Compute in place forward FFT */
  cufftExecC2C (plan, r_complex_d, r_complex_d, CUFFT_FORWARD);

/* Solve Poisson equation in Fourier space */
  solve_poisson<<<dimGrid, dimBlock>>> (r_complex_d, kx_d, ky_d,N);

/* Compute in place inverse FFT */
  cufftExecC2C (plan, r_complex_d, r_complex_d, CUFFT_INVERSE);

 /* Copy the solution back to a real array and apply scaling ( an FFT followed by
      iFFT will give you back the same array times the length of the transform) */
  scale = 1.f / ( (float) N * (float) N );
  complex2real_scaled<<<dimGrid, dimBlock>>> (r_d, r_complex_d, N, scale);
```

Code walk-through (step 11)

```
/*Transfer data from device to host  with
   cudaMemcpy(target, source, size, direction)*/
  cudaMemcpy (r  , r_d   , sizeof(float)*N*N, cudaMemcpyDeviceToHost);

/* Destroy  plan and clean up memory on device*/
   cufftDestroy( plan);
   cudaFree(r_complex_d);
   …….
   cudaFree(kx_d);
```


real2complex

```
/*Copy real data to complex data */

  __global__ void real2complex (float *a,  cufftComplex *c, int N)
{
      /* compute idx and idy, the location of the element in the original NxN array */
      int idx = blockId.x*blockDim.x+threadIdx.x;
      int idy = blockId.y*blockDim.y+threadIdx.y;

      if ( idx < N && idy <N)
            {
             int index = idx + idy*N;
             c[index].x = a[index];
             c[index].y = 0.f;
            }
}
```



solve_poisson

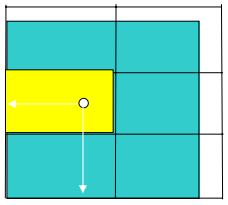
```
__global__ void solve_poisson (cufftComplex *c, float *kx, float *ky, int N)
{
    /* compute idx and idy, the location of the element in the original NxN
    array */
    int idx = blockId.x*blockDim.x+threadIdx.x;
    int idy = blockId.y*blockDim.y+threadIdx.y;

    if ( idx < N && idy <N)
        {
         int index = idx + idy*N;
         float scale =  -  ( kx[idx]*kx[idx] + ky[idy]*ky[idy] );
         if ( idx ==0 && idy == 0 ) scale =1.f;
         scale = 1.f / scale;
         c[index].x *= scale;
         c[index].y *= scale;
        }
}
```

$$\hat{\phi} = -\frac{\hat{r}}{(k_x^2 + k_y^2)}$$

complex2real_scaled

```
/*Copy real part of complex data into real array and apply scaling */

__global__ void complex2real_scaled (cufftComplex *c, float *a, int N,
                                     float scale)
{
    /* compute idx and idy, the location of the element in the original NxN array */
    int idx = blockId.x*blockDim.x+threadIdx.x;
    int idy = blockId.y*blockDim.y+threadIdx.y;

    if ( idx < N && idy <N)
        {
         int index = idx + idy*N;
         a[index] = scale*c[index].x ;
         }
}
```

idy



idx

Compile and run poisson_1

- **Compile the example poisson_1.cu:**

  nvcc –O3 –o poisson_1 poisson_1.cu \\
  -I/usr/local/cuda/include –L/usr/local/cuda/lib -lcufft –lcudart

- **Run the example**

  ./poisson_1 -N64
  Poisson solver on a domain 64 x 64
  dimBlock 32 16 (512 threads)
  dimGrid 2 4
  L2 error 9.436995e-08:
  Time 0.000569:
  Time I/O 0.000200 (0.000136 + 0.000064):
  Solution at (32,32)
  computed=0.975879 reference=0.975882

- **Reference values from MATLAB:**

  N=64
  Solution at (32,32): computed= 0.975879 reference= 0.975882
  Linf err=2.404194e-05 L2 norm err = 9.412790e-08

Profiling

Profiling the function calls in CUDA is very easy.
It is controlled via environment variables:

- **CUDA_PROFILE: to enable or disable**
  - **1 (enable profiler)**
  - **0 (default, no profiler)**
- **CUDA_PROFILE_LOG: to specify the filename**
  - **If set, it will write to "filename"**
  - **If not set, it will write to cuda_profile.log**
- **CUDA_PROFILE_CSV: control the format**
  - **1 (enable comma separated file)**
  - **0 (disable comma separated file)**

Profiler output from Poisson_1

./poisson_1 –N1024

method=[memcopy] gputime=[1427.200]
method=[memcopy] gputime=[10.112]
method=[memcopy] gputime=[9.632]

method=[real2complex] gputime=[1654.080] cputime=[1702.000] occupancy=[0.667]

method=[c2c_radix4] gputime=[8651.936] cputime=[8683.000] occupancy=[0.333]
method=[transpose] gputime=[2728.640] cputime=[2773.000] occupancy=[0.333]
method=[c2c_radix4] gputime=[8619.968] cputime=[8651.000] occupancy=[0.333]
method=[c2c_transpose] gputime=[2731.456] cputime=[2762.000] occupancy=[0.333]

method=[solve_poisson] gputime=[6389.984] cputime=[6422.000] occupancy=[0.667]

method=[c2c_radix4] gputime=[8518.208] cputime=[8556.000] occupancy=[0.333]
method=[c2c_transpose] gputime=[2724.000] cputime=[2757.000] occupancy=[0.333]
method=[c2c_radix4] gputime=[8618.752] cputime=[8652.000] occupancy=[0.333]
method=[c2c_transpose] gputime=[2767.840] cputime=[5248.000] occupancy=[0.333]

method=[complex2real_scaled] gputime=[2844.096] cputime=[3613.000] occupancy=[0.667]

method=[memcopy] gputime=[2461.312]

Improving performances

- **Use pinned memory to improve CPU/GPU transfer time:**

```
#ifdef PINNED
      cudaMallocHost((void **) &r,sizeof(float)*N*N); // rhs, 2D array
#else
      r  = (float *) malloc(sizeof(float)*N*N); // rhs, 2D array
#endif
```

```
$ ./poisson_1
Poisson solver on a domain  1024 x 1024
Total Time   : 69.929001 (ms)
Solution Time: 60.551998 (ms)
Time I/O     : 8.788000 (5.255000 + 3.533000) (ms)

$ ./poisson_1_pinned
Poisson solver on a domain  1024 x 1024
Total Time   : 66.554001 (ms)
Solution Time: 60.736000 (ms)
Time I/O     : 5.235000 (2.027000 + 3.208000) (ms)
```


Additional improvements

- Use shared memory for the arrays kx and ky in solve_poisson
- Use fast integer operations (__umul24)

solve_poisson (with shared memory)

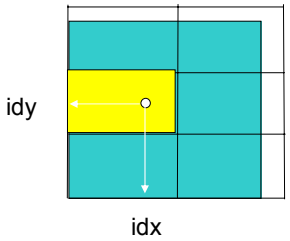
```
__global__ void solve_poisson (cufftComplex *c, float *kx, float *ky, int N)
{
      unsigned int idx   = __umul24(blockIdx.x,blockDim.x)+threadIdx.x;
      unsigned int idy   = __umul24(blockIdx.y,blockDim.y)+threadIdx.y;
// use shared memory to minimize multiple access to same k values
     __shared__ float kx_s[BLOCK_WIDTH], ky_s[BLOCK_HEIGHT]
      if (threadIx.x < 1) kx_s[threadIdx.x] = kx[idx];
      if (threadIx.y < 1) ky_s[threadIdx.y] = ky[idy];
      __syncthreads();
       if ( idx < N && idy <N)
            {
            unsigned int index = idx +__umul24(idy ,N);
            float scale =  -  ( kx_s[threadIdx.x]*kx_s[threadIdx.x]
                           +    ky_s[threadIdy.y]*ky_s[threadIdy.y] );
            if ( idx ==0 && idy == 0 ) scale =1.f;
            scale = 1.f / scale;
             c[index].x *= scale;
             c[index].y*= scale;
            }
}
```


Profiler output from Poisson_2

```
./poisson_2 –N1024 –x16 –y16

method=[ memcopy ] gputime=[ 1426.048 ]
method=[ memcopy ] gputime=[ 9.760 ]
method=[ memcopy ] gputime=[ 9.472 ]

method=[ real2complex ] gputime=[ 1611.616 ] cputime=[ 1662.000 ] occupancy=[ 0.667 ] (was 1654)

method=[ c2c_radix4 ] gputime=[ 8658.304 ] cputime=[ 8689.000 ] occupancy=[ 0.333 ]
method=[ c2c_transpose ] gputime=[ 2731.424 ] cputime=[ 2763.000 ] occupancy=[ 0.333 ]
method=[ c2c_radix4 ] gputime=[ 8622.048 ] cputime=[ 8652.000 ] occupancy=[ 0.333 ]
method=[ c2c_transpose] gputime=[ 2738.592 ] cputime=[ 2770.000 ] occupancy=[ 0.333 ]

method=[ solve_poisson] gputime=[ 2760.192 ] cputime=[ 2792.000 ] occupancy=[ 0.667 ] (was 6389)

method=[ c2c_radix4 ] gputime=[ 8517.952 ] cputime=[ 8550.000 ] occupancy=[ 0.333 ]
method=[ c2c_transpose] gputime=[ 2729.632 ] cputime=[ 2766.000 ] occupancy=[ 0.333 ]
method=[ c2c_radix4 ] gputime=[ 8621.024 ] cputime=[ 8653.000 ] occupancy=[ 0.333 ]
method=[ c2c_transpose] gputime=[ 2770.912 ] cputime=[ 5252.000 ] occupancy=[ 0.333 ]

method=[ complex2real_scaled ] gputime=[ 2847.008 ] cputime=[ 3616.000 ] occupancy=[ 0.667 ]
                                        ???????
method=[ memcopy ] gputime=[ 2459.872 ]
```


complex2real_scaled (fast version)

```
__global__ void complex2real_scaled (cufftComplex *c, float *a, int N, float
    scale)
{
    /* compute idx and idy, the location of the element in the original NxN array */
    int idx = blockId.x*blockDim.x+threadIdx.x;
    int idy = blockId.y*blockDim.y+threadIdx.y;
    volatile float2 c2;
        if ( idx < N && idy <N)
        {
         int index = idx + idy*N;
         c2.x= c[index].x;
         c2.y= c[index].y;
         a[index] = scale*c2.x ;
         }
}
```



From the ptx file, we discover that the compiler is optimizing out the vector load which prevents memory coalescing. Use volatile to force vector load

Profiler output from Poisson_3

```
method=[ memcopy ] gputime=[ 1427.808 ]
method=[ memcopy ] gputime=[ 9.856 ]
method=[ memcopy ] gputime=[ 9.600 ]

method=[ real2complex] gputime=[ 1614.144 ] cputime=[ 1662.000 ] occupancy=[ 0.667 ]

method=[ c2c_radix4]       gputime=[ 8656.800 ] cputime=[ 8688.000 ] occupancy=[ 0.333 ]
method=[ c2c_transpose] gputime=[ 2727.200 ] cputime=[ 2758.000 ] occupancy=[ 0.333 ]
method=[ c2c_radix4 ]      gputime=[ 8607.616 ] cputime=[ 8638.000 ] occupancy=[ 0.333 ]
method=[ c2c_transpose] gputime=[ 2729.888 ] cputime=[ 2761.000 ] occupancy=[ 0.333 ]

method=[ solve_poisson ] gputime=[ 2762.656 ] cputime=[ 2794.000 ] occupancy=[ 0.667 ]

method=[ c2c_radix4 ]      gputime=[ 8514.720 ] cputime=[ 8547.000 ] occupancy=[ 0.333 ]
method=[ c2c_transpose] gputime=[ 2724.192 ] cputime=[ 2760.000 ] occupancy=[ 0.333 ]
method=[ c2c_radix4 ]      gputime=[ 8620.064 ] cputime=[ 8652.000 ] occupancy=[ 0.333 ]
method=[ c2c_transpose] gputime=[ 2773.920 ] cputime=[ 4270.000 ] occupancy=[ 0.333 ]

method=[ complex2real_scaled ] gputime=[ 1524.992 ] cputime=[ 1562.000 ] occupancy=[ 0.667 ]

method=[ memcopy ] gputime=[ 2468.288 ]
```


Performance improvement

	Non-pinned memory	Pinned memory
Initial implementation (r2c, poisson, c2r)	67ms (10.8ms)	63ms
+Shared memory +Fast integer mul	63.4ms (7.1ms)	59.4ms
+Coalesced read in c2r	62.1ms (5.8ms)	58.2ms

Tesla C870, pinned memory, optimized version: 10.4ms

S05: High Performance Computing with CUDA

Accelerating MATLAB with CUDA

Overview

MATLAB can be easily extended via MEX files to take advantage of the computational power offered by the latest NVIDIA GPUs (GeForce 8800, Quadro FX5600, Tesla).

Programming the GPU for computational purposes was a very cumbersome task before CUDA. Using CUDA, it is now very easy to achieve impressive speed-up with minimal effort.

MEX file

- Even though MATLAB is built on many well-optimized libraries, some functions can perform better when written in a compiled language (e.g. C and Fortran).
- MATLAB provides a convenient API for interfacing code written in C and FORTRAN to MATLAB functions with MEX files.
- MEX files could be used to exploit multi-core processors with OpenMP or threaded codes or like in this case to offload functions to the GPU.

NVMEX

- Native MATLAB script cannot parse CUDA code
- New MATLAB script nvmex.m compiles CUDA code (.cu) to create MATLAB function files
- Syntax similar to original mex script:

```
>> nvmex –f nvmexopts.bat filename.cu –IC:\cuda\include
     –LC:\cuda\lib -lcudart
```

Available for Windows and Linux from:
http://developer.nvidia.com/object/matlab_cuda.html

Mex files for CUDA

A typical mex file will perform the following steps:

1. Convert from double to single precision
2. Rearrange the data layout for complex data
3. Allocate memory on the GPU
4. Transfer the data from the host to the GPU
5. Perform computation on GPU (library, custom code)
6. Transfer results from the GPU to the host
7. Rearrange the data layout for complex data
8. Convert from single to double
9. Clean up memory and return results to MATLAB

Some of these steps will go away with new versions of the library (2,7) and new hardware (1,8)

CUDA MEX example

Additional code in MEX file to handle CUDA

```
/*Parse input, convert to single precision and to interleaved complex format */
      .....
/* Allocate array on the GPU */
      cufftComplex *rhs_complex_d;
      cudaMalloc( (void **) &rhs_complex_d,sizeof(cufftComplex)*N*M);
/* Copy input array in interleaved format to the GPU */
      cudaMemcpy( rhs_complex_d, input_single, sizeof(cufftComplex)*N*M,
                                          cudaMemcpyHostToDevice);
/* Create plan for CUDA FFT  NB: transposing dimensions*/
      cufftPlan2d(&plan, N, M, CUFFT_C2C) ;
/* Execute FFT on GPU */
      cufftExecC2C(plan, rhs_complex_d, rhs_complex_d, CUFFT_INVERSE) ;
/* Copy result back to host */
      cudaMemcpy( input_single, rhs_complex_d, sizeof(cufftComplex)*N*M,
                                          cudaMemcpyDeviceToHost);
/* Clean up memory and plan on the GPU */
      cufftDestroy(plan); cudaFree(rhs_complex_d);
/*Convert back to double precision and to split complex format */
```


Initial study

- Focus on 2D FFTs.
- FFT-based methods are often used in single precision (for example in image processing)
- Mex files to overload MATLAB functions, no modification between the original MATLAB code and the accelerated one.
- Application selected for this study:
  solution of the Euler equations in vorticity form using a pseudo-spectral method.

Implementation details:

Case A) FFT2.mex and IFFT2.mex

Mex file in C with CUDA FFT functions.

Standard mex script could be used.

Overall effort: few hours

Case B) Szeta.mex: Vorticity source term written in CUDA

Mex file in CUDA with calls to CUDA FFT functions.

Small modifications necessary to handle files with a .cu suffix

Overall effort: ½ hour (starting from working mex file for 2D FFT)

Configuration

Hardware:

AMD Opteron 250 with 4 GB of memory

NVIDIA GeForce 8800 GTX

Software:

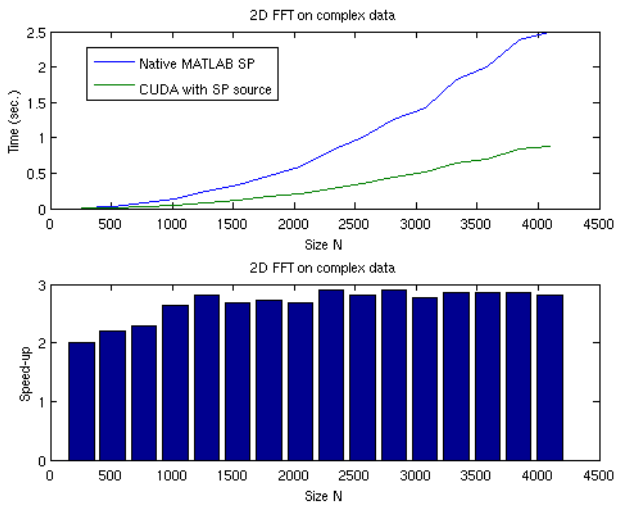
Windows XP and Microsoft VC8 compiler

RedHat Enterprise Linux 4 32 bit, gcc compiler

MATLAB R2006b

CUDA 1.0

FFT2 performance



Vorticity source term

http://www.amath.washington.edu/courses/571-winter-2006/matlab/Szeta.m

```
function S = Szeta(zeta,k,nu4)

% Pseudospectral calculation of vorticity source term
% S = -(- psi_y*zeta_x + psi_x*zeta_y) + nu4*del^4 zeta
% on a square periodic domain, where zeta = psi_xx + psi_yy is an NxN matrix
% of vorticity and k is vector of Fourier wavenumbers in each direction.
% Output is an NxN matrix of S at all pseudospectral gridpoints
      zetahat = fft2(zeta);
      [KX KY] = meshgrid(k,k);
% Matrix of (x,y) wavenumbers corresponding
% to Fourier mode (m,n)
      del2 = -(KX.^2 + KY.^2);
      del2(1,1) = 1; % Set to nonzero to avoid division by zero when inverting
% Laplacian to get psi
      psihat = zetahat./del2;
      dpsidx = real(ifft2(1i*KX.*psihat));
      dpsidy = real(ifft2(1i*KY.*psihat));
      dzetadx = real(ifft2(1i*KX.*zetahat));
      dzetady = real(ifft2(1i*KY.*zetahat));
      diff4 = real(ifft2(del2.^2.*zetahat));
      S = -(-dpsidy.*dzetadx + dpsidx.*dzetady) - nu4*diff4;
```


Caveats

The current CUDA FFT library only supports interleaved format for complex data while MATLAB stores all the real data followed by the imaginary data.

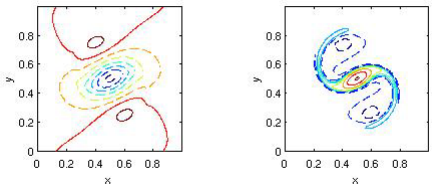
Complex to complex (C2C) transforms used

The accelerated computations are not taking advantage of the symmetry of the transforms.

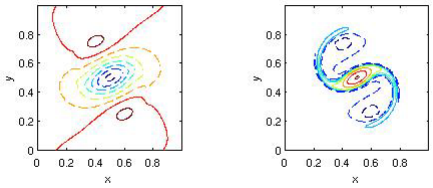
The current GPU hardware only supports single precision (double precision will be available in the next generation GPU towards the end of the year). Conversion to/from single from/to double is consuming a significant portion of wall clock time.

Advection of an elliptic vortex

256x256 mesh, 512 RK4 steps, Linux, MATLAB file
http://www.amath.washington.edu/courses/571-winter-2006/matlab/FS_vortex.m



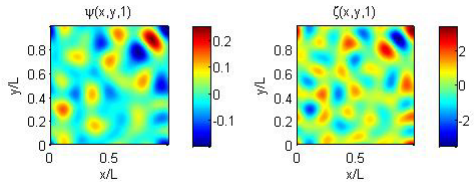
MATLAB
168 seconds



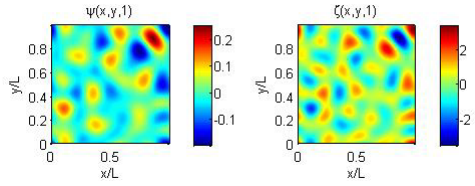
MATLAB with CUDA
(single precision FFTs)
14.9 seconds (11x)

Pseudo-spectral simulation of 2D Isotropic turbulence.

512x512 mesh, 400 RK4 steps, Windows XP, MATLAB file
http://www.amath.washington.edu/courses/571-winter-2006/matlab/FS_2Dturb.m

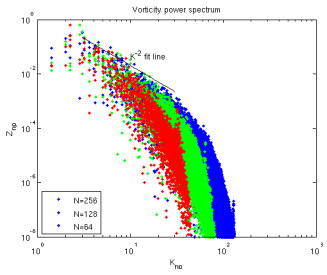


MATLAB
992 seconds

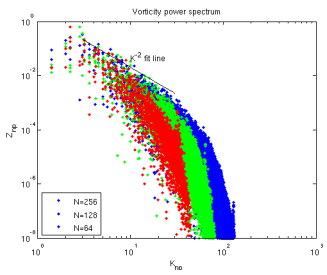


MATLAB with CUDA
(single precision FFTs)
93 seconds

- **Power spectrum of vorticity is very sensitive to fine scales. Result from original MATLAB run and CUDA accelerated one are in excellent agreement**



MATLAB run



CUDA accelerated MATLAB run

Timing details

1024x1024 mesh, 400 RK4 steps on Windows, 2D isotropic turbulence

	Runtime Opteron 250	Speed up	Runtime Opteron 2210	Speed up
PCI-e Bandwidth: Host to/from device	1135 MB/s 1003 MB/s		1483 MB/s 1223 MB/s	
Standard MATLAB	8098 s		9525s	
Overload FFT2 and IFFT2	4425 s	1.8x	4937s	1.9x
Overload Szeta	735 s	11.x	789s	12.X
Overload Szeta , FFT2 and IFFT2	577 s	14.x	605s	15.7x

Conclusion

- Integration of CUDA is straightforward as a MEX plug-in
- No need for users to leave MATLAB to run big simulations:
  - high productivity
- Relevant speed-ups even for small size grids
- Plenty of opportunities for further optimizations