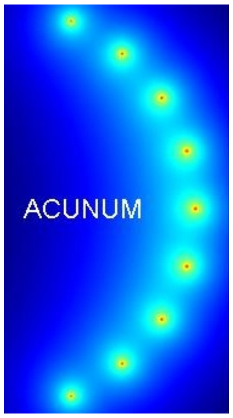
C++/CUDA Implementation of the Weeks Method for Numerical Laplace Transform Inversion



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May 17, 2011

Introduction

While tables of forward and inverse Laplace transforms are commonly used for textbook exercises, real world engineering

$$f(t) = \frac{1}{2\pi i}\int_{\Gamma} e^{st}F(s)ds \qquad F(s) = \int_{-\infty}^{\infty} e^{-st}f(t)dt$$

and scientific problems often present Laplace space solutions F(s) that can not be inverted by standard methods. The numerical inversion of the Laplace transform is an obvious approach to mitigating this problem. Numerical inversion is however known to be a paradigm of an exponentially ill-posed problem [2] and thus requires careful consideration. Many algorithms have been presented to perform the numerical inversion [3]. Implemented here is one of the more well known, the Weeks method [6]. This software has been written to take advantage of the parallel computations that are available on modern graphics processing units.

Description of the Weeks Method

The Weeks method involves a Laguerre polynomial expansion of the time domain function f(t).

$$L_n(x) = \frac{e^x}{n!}\frac{d^n}{dx^n}(x^n e^{-x})$$

$$f(t) \approx \sum_{n=0}^{N-1} a_n e^{(\sigma-b)t} L_n(2bt)$$

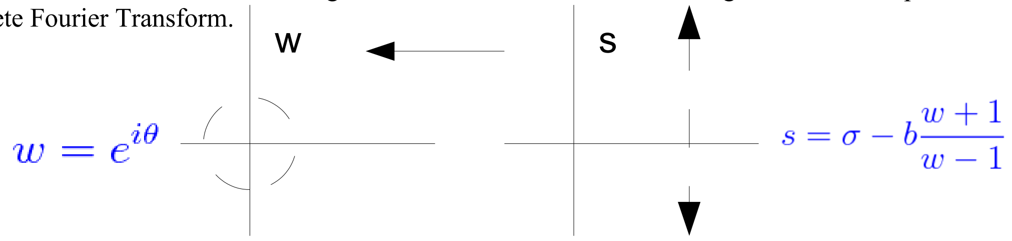
The expansions coefficients are dependent on the Laplace space function F(s) where *s* is a complex variable.

$$a_n = a_n(F(s), \sigma, b)$$

The coefficients are computed by performing an contour integration in the w-plane on a unit circle that encloses the singularities of the mapped F(w).

$$a_n = \frac{1}{2\pi i}\int_{|w|=1} w^{-(n+1)}\frac{2b}{1-w}F\left(\sigma - b\frac{w+1}{w-1}\right)dw$$

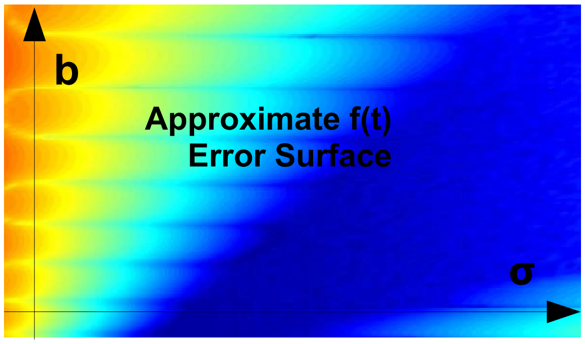
By sampling F(w) on the unit circle at a uniform angular distribution, the numerical integration via a midpoint rule is equivalent to a discrete Fourier Transform.



The core computation of the Weeks method Laguerre expansion is thus to compute the coefficients via a Fast Fourier transform of samples of the Laplace space function F(s) that has been mapped with a Moebius transformation from the *s* to the *w* plane. The choice of the mapping parameters is obviously critical.

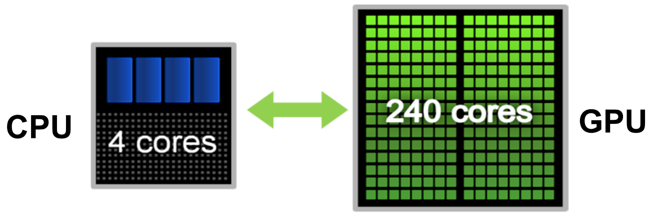
Parameter Selection

The Weeks method includes two free positive scaling parameters (σ, b). By appropriately choosing these parameters, an accurate inversion can be obtained. The parameter selection can be accomplished from a minimization of an absolute error estimate E(t; σ, b) for the approximate f(t). The calculation of the error estimate involves the determination of the expansion coefficients and thus a fast Fourier transform for each (σ,b) pair. This direct global error estimate minimization is a computationally intensive approach. It is however a robust method [5] and the reliability of the inversion is paramount.



GPU Acceleration

New in this software is the use of graphics processing units [GPU] to calculate in parallel the error estimate for each (σ, b) pair [4]. The code is fundamentally a standard C++ class called *WeeksNLAP*. However, for the coefficient computations, NVIDIA's Compute Unified Device Architecture [CUDA] is used [1] . With CUDA, C kernel functions are included to implement the parallel sampling and Fast Fourier transforms on the GPU. This error estimation problem is well suited to GPU implementation in that it involves multiple executions of the same instructions. The graphics card contains many more cores than the central processing unit and is therefore able to compute in parallel far more of these similar commands. To be concise, the C-GPU functions are primarily used to perform in parallel the F(s) sampling and FFT for each (σ, b). From these, a minimum error estimate is obtained and an optimal (σ, b) pair used in the Weeks expansion.



User Interface

To assist the user, the interface to the code has two been reduced to two files.

1. UserFs.txt Provides the definition of F(s) to invert
2. UserParameters.txt Provides the user controlled computation parameters

Currently, the code must be recompiled for each F(s) expression that the user defines in UserFs.txt. F(s) must also be written using CUDA's cuDoubleComplex variables.

The parameters file UserParameters.txt is read in the WeeksNLAP class constructor when an object is created. The format of the file can not be changed. The contents are described in this table:

User Input Parameters			
Type	**Parameter**	**Description**	**Comment**
integer	LengthTimes	Number of inversion times.	
double	*Timevec	The inversion times.	This vector must have a length equal to LengthTimes
double	*RelErrorTol	Relative error tolerance for the inversions.	0.x is an x% relative error
integer	SearchSwitch	A switch to allow the user to directly specify the (σ, b) parameters or allow the code to perform an internal search. 1-search for parameters	The user can specify the scaling parameters directly without a search.

		0-user defined parameters	
integer	LengthLag	The length of the NLag vector.	
integer	*NLag	The number of Laguerre expansion coefficients.	Powers of 2
double	sigmaUser	A user defined σ value for each time.	if SearchSwitch =0
double	bUser	A user defined b value for each time.	if SearchSwitch =0
integer	Lengthtol	The length of the tolerances vectors tols & tolb.	if SearchSwitch = 1
double	sigmin	The minimum σ value searched.	if SearchSwitch = 1
double	sigmax	The maximum σ value searched.	if SearchSwitch = 1
double	*tols	The σ grid resolution.	if SearchSwitch = 1
double	bmax	The maximum b value searched.	if SearchSwitch = 1
double	*tolb	The b grid resolution.	if SearchSwitch = 1

The relative error tolerances in the vector *RelErrorTol* are specified by the user for each time in the vector *Timevec*. This code refines the f(t) approximations at each time with increasing σ *tols* and b *tolb* resolutions until an internal estimate of the relative error is below the user requested tolerance or the maximum number of iterations is reached. In either case, a output flag indicates if the predicted estimate is below the tolerance.

The code generates an array of output structures *arrayOutput* for each inversion time. In addition to the approximate f(t), each structure contains the data listed in this table:

Code Generated Output Data			
Type	**Data**	**Description**	**Comment**
double	time	Inversion time supplied by the user.	
double complex	Invertf	Approximate f(t)	
double	sigmaP	σ used in the inversion	from the search or defined by the user
double	bP	b used in the inversion	from the search or defined by the user
double	AbsTotalError	Estimated absolute truncation and round-off error	0.x is an x% relative error
double	RelTotalError	Estimated relative truncation and round-off error using the approximate f(t)	0.x is an x% relative error
integer	ToleranceMetFlag	A flag to indicate if the estimated relative error is below the user specified tolerance. 1=Failure 0=Success	

The input parameters and output results are written to the screen via an optional display function.

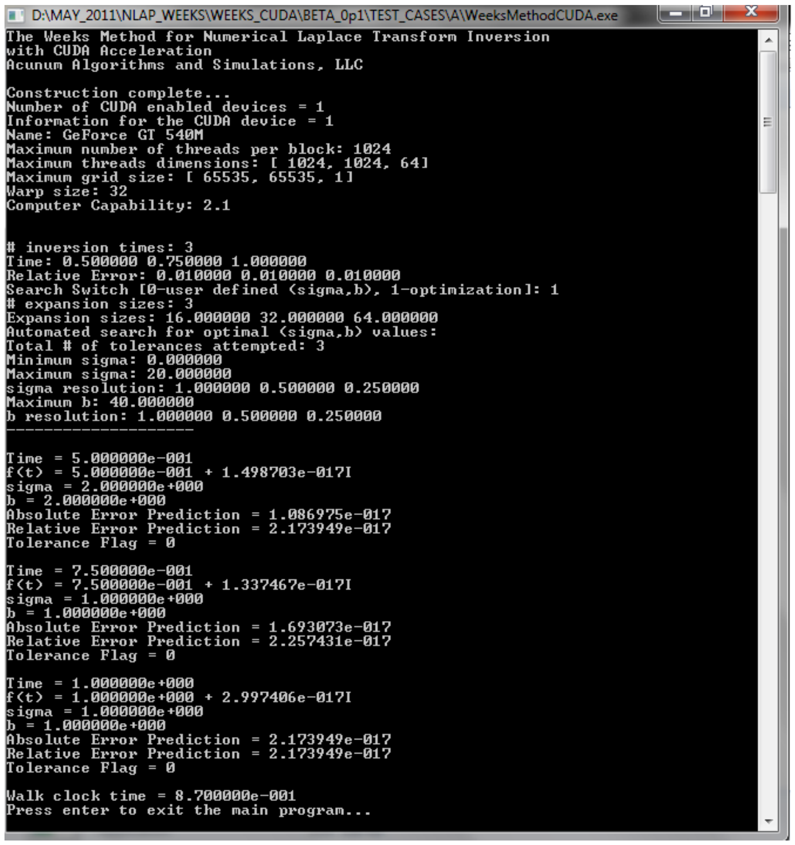
Example Use

Four default examples are coded in the UserFs.txt file. Also supplied are the corresponding input parameter files. These examples have been used to verify the code . They are also some of the test cases in the examples script for the MATLAB implementation by Acunum of this GPU accelerated Weeks method approach [4].

A) The first example is a very simple case where the time domain function is the time.

$$F(s) = 1/s^2 \leftrightarrow f(t) = t$$

The output of the code is captured here:



```
D:\MAY_2011\NLAP_WEEKS\WEEKS_CUDA\BETA_0p1\TEST_CASES\A\WeeksMethodCUDA.exe
The Weeks Method for Numerical Laplace Transform Inversion
with CUDA Acceleration
Acunum Algorithms and Simulations, LLC

Construction complete...
Number of CUDA enabled devices = 1
Information for the CUDA device = 1
Name: GeForce GT 540M
Maximum number of threads per block: 1024
Maximum threads dimensions: [ 1024, 1024, 64]
Maximum grid size: [ 65535, 65535, 1]
Warp size: 32
Computer Capability: 2.1


# inversion times: 3
Time: 0.500000 0.750000 1.000000
Relative Error: 0.010000 0.010000 0.010000
Search Switch [0-user defined (sigma,b), 1-optimization]: 1
# expansion sizes: 3
Expansion sizes: 16.000000 32.000000 64.000000
Automated search for optimal (sigma,b) values:
Total # of tolerances attempted: 3
Minimum sigma: 0.000000
Maximum sigma: 20.000000
sigma resolution: 1.000000 0.500000 0.250000
Maximum b: 40.000000
b resolution: 1.000000 0.500000 0.250000
--------------------

Time = 5.000000e-001
f(t) = 5.000000e-001 + 1.498703e-017I
sigma = 2.000000e+000
b = 2.000000e+000
Absolute Error Prediction = 1.086975e-017
Relative Error Prediction = 2.173949e-017
Tolerance Flag = 0

Time = 7.500000e-001
f(t) = 7.500000e-001 + 1.337467e-017I
sigma = 1.000000e+000
b = 1.000000e+000
Absolute Error Prediction = 1.693073e-017
Relative Error Prediction = 2.257431e-017
Tolerance Flag = 0

Time = 1.000000e+000
f(t) = 1.000000e+000 + 2.997406e-017I
sigma = 1.000000e+000
b = 1.000000e+000
Absolute Error Prediction = 2.173949e-017
Relative Error Prediction = 2.173949e-017
Tolerance Flag = 0

Walk clock time = 8.700000e-001
Press enter to exit the main program...
```

The estimated error is clearly at the limits of double precision accuracy.

The total execution time in seconds for the code to invert at sixteen times is shown in the following table as a function of the number of expansion coefficients and grid resolution. The code is run with σ from [0,20) and b from [0,40).

		σ resolution		
N coefficients	**b resolution**	**1**	**0.5**	**0.25**
16	**1**	2.05	3.28	5.75
	0.5	3.28	5.75	10.7
	0.25	5.77	10.69	20.56
32	**1**	3.3	5.77	10.73
	0.5	5.77	10.72	20.63
	0.25	10.73	20.61	40.42
64	**1**	5.79	10.75	20.67
	0.5	10.75	20.66	40.5
	0.25	20.67	40.48	80.15

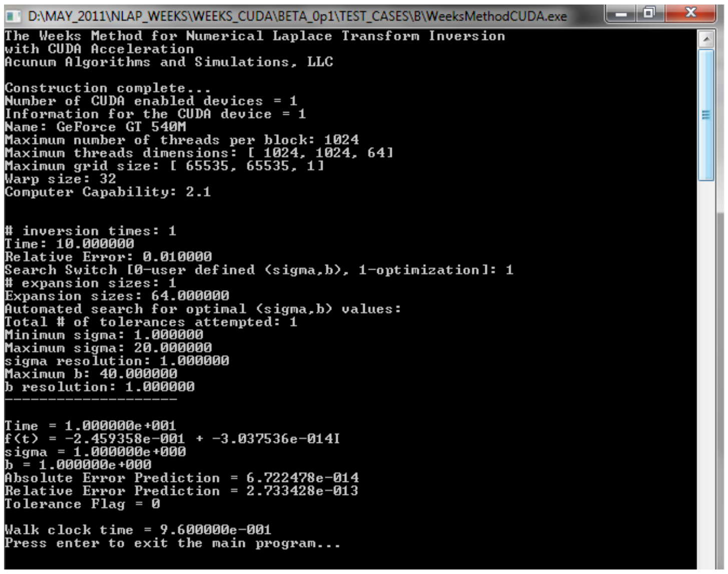
The run time doubles with double resolution.

Focusing on the GPU implemented computations yields the run times in the next table. These numbers are in seconds and for the inversion at a single time. They were captured using the *cudaEvent* timing mechanism in CUDA. An observation from this data is that the parallel FFT on the GPU is only a fraction of the total run time. Rather, the F(s) sampling and coefficients computations are much more time consuming.

N	**16**	**32**	**64**	**64**	**64**
σ resolution	**0.25**	**0.25**	**0.25**	**0.25**	**0.25**
b resolution	**0.25**	**0.25**	**0.25**	**0.5**	**1**
Sample F(s)	0.497690	0.995320	1.990530	0.995330	0.497640
Shift F(s) ordering	0.081770	0.164090	0.328660	0.164240	0.082110
FFT	0.002260	0.01	0.013970	0.007030	0.003510
Coefficient Computation	0.290130	0.583560	1.171440	0.585850	0.292820
Error Estimation	0.067080	0.131620	0.261220	0.130860	0.065530
Total GPU	0.938930	1.879970	3.765820	1.883310	0.941610
Wall Clock	1.860000	3.100000	5.590000	3.100000	1.87000

B) The second example involves a numerical inversion to obtain the zeroth Bessel function. The function's value at t=10 is -0.245935764. The screenshot below demonstrates that the code determined (σ, b) values that accurately inverted F(s).

$$F(s) = \frac{1}{\sqrt{(s^2+1)}} \leftrightarrow f(t) = J_0(t)$$


D:\MAY_2011\NLAP_WEEKS\WEEKS_CUDA\BETA_0p1\TEST_CASES\B\WeeksMethodCUDA.exe

```
The Weeks Method for Numerical Laplace Transform Inversion
with CUDA Acceleration
Acunum Algorithms and Simulations, LLC

Construction complete...
Number of CUDA enabled devices = 1
Information for the CUDA device = 1
Name: GeForce GT 540M
Maximum number of threads per block: 1024
Maximum threads dimensions: [ 1024, 1024, 64]
Maximum grid size: [ 65535, 65535, 1]
Warp size: 32
Computer Capability: 2.1

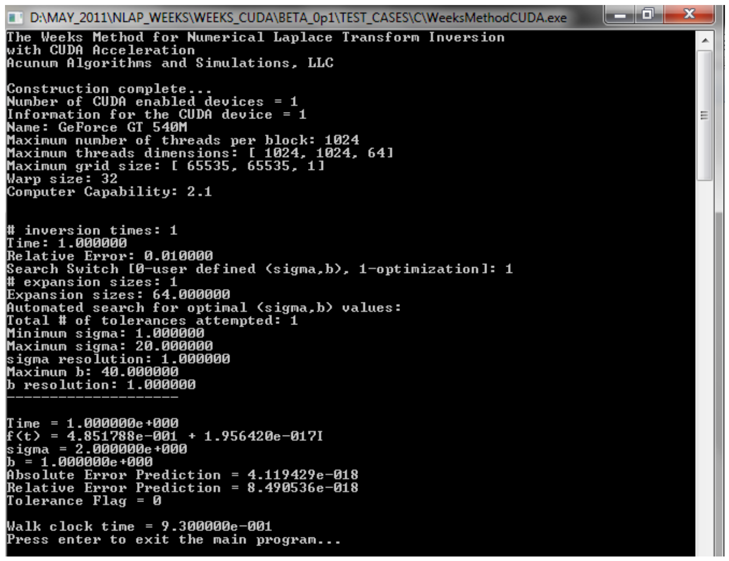

# inversion times: 1
Time: 10.000000
Relative Error: 0.010000
Search Switch [0-user defined (sigma,b), 1-optimization]: 1
# expansion sizes: 1
Expansion sizes: 64.000000
Automated search for optimal (sigma,b) values:
Total # of tolerances attempted: 1
Minimum sigma: 1.000000
Maximum sigma: 20.000000
sigma resolution: 1.000000
Maximum b: 40.000000
b resolution: 1.000000
--------------------

Time = 1.000000e+001
f(t) = -2.459358e-001 + -3.037536e-014I
sigma = 1.000000e+000
b = 1.000000e+000
Absolute Error Prediction = 6.722478e-014
Relative Error Prediction = 2.733428e-013
Tolerance Flag = 0

Walk clock time = 9.600000e-001
Press enter to exit the main program...
```

C) The third example can be analytically inverted using tables and partial fractions. The expression for f(t) is purely harmonic and has a value at t=1 of 0.4851788474. Again, one sees in the screenshot that the code accurately captured the correct approximate f(t).

$$F(s) = \frac{1}{s(s^2+9/25)} \leftrightarrow f(t) = (25/9)(1-\cos(3t/5))$$



```
D:\MAY_2011\NLAP_WEEKS\WEEKS_CUDA\BETA_0p1\TEST_CASES\C\WeeksMethodCUDA.exe
The Weeks Method for Numerical Laplace Transform Inversion
with CUDA Acceleration
Acunum Algorithms and Simulations, LLC

Construction complete...
Number of CUDA enabled devices = 1
Information for the CUDA device = 1
Name: GeForce GT 540M
Maximum number of threads per block: 1024
Maximum threads dimensions: [ 1024, 1024, 64]
Maximum grid size: [ 65535, 65535, 1]
Warp size: 32
Computer Capability: 2.1

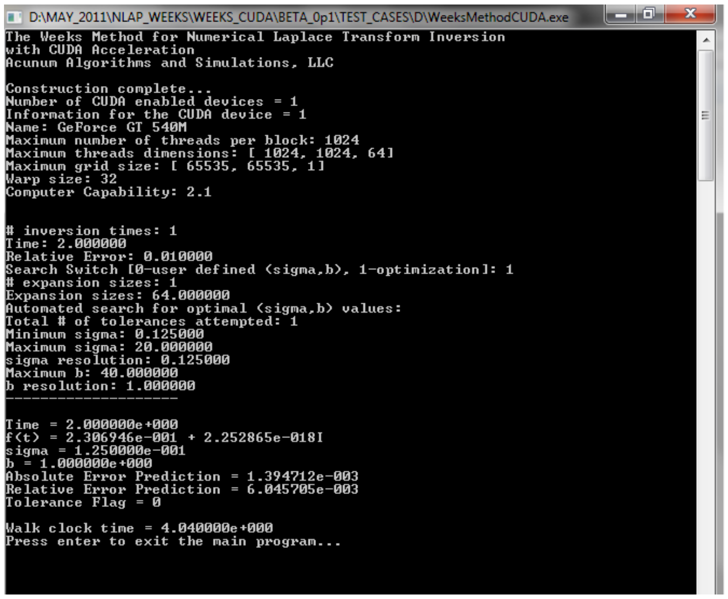

# inversion times: 1
Time: 1.000000
Relative Error: 0.010000
Search Switch [0-user defined (sigma,b), 1-optimization]: 1
# expansion sizes: 1
Expansion sizes: 64.000000
Automated search for optimal (sigma,b) values:
Total # of tolerances attempted: 1
Minimum sigma: 1.000000
Maximum sigma: 20.000000
sigma resolution: 1.000000
Maximum b: 40.000000
b resolution: 1.000000
--------------------

Time = 1.000000e+000
f(t) = 4.851788e-001 + 1.956420e-017I
sigma = 2.000000e+000
b = 1.000000e+000
Absolute Error Prediction = 4.119429e-018
Relative Error Prediction = 8.490536e-018
Tolerance Flag = 0

Walk clock time = 9.300000e-001
Press enter to exit the main program...
```

D) This fourth example involves fraction exponents. The time domain function includes a coefficient that is defined in terms of the Gamma function. At time t=2, the time domain function is 0.23202351899818. The code accurately estimates this value to within 0.6% relative error.

$$F(s) = \frac{1}{(s+3/5)^{9/11}} \leftrightarrow f(t) = \frac{1}{t^{2/11}e^{3t/5}\Gamma(9/11)}$$



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D:\MAY_2011\NLAP_WEEKS\WEEKS_CUDA\BETA_0p1\TEST_CASES\D\WeeksMethodCUDA.exe
The Weeks Method for Numerical Laplace Transform Inversion
with CUDA Acceleration
Acunum Algorithms and Simulations, LLC

Construction complete...
Number of CUDA enabled devices = 1
Information for the CUDA device = 1
Name: GeForce GT 540M
Maximum number of threads per block: 1024
Maximum threads dimensions: [ 1024, 1024, 64]
Maximum grid size: [ 65535, 65535, 1]
Warp size: 32
Computer Capability: 2.1


# inversion times: 1
Time: 2.000000
Relative Error: 0.010000
Search Switch [0-user defined (sigma,b), 1-optimization]: 1
# expansion sizes: 1
Expansion sizes: 64.000000
Automated search for optimal (sigma,b) values:
Total # of tolerances attempted: 1
Minimum sigma: 0.125000
Maximum sigma: 20.000000
sigma resolution: 0.125000
Maximum b: 40.000000
b resolution: 1.000000
--------------------

Time = 2.000000e+000
f(t) = 2.306946e-001 + 2.252865e-018I
sigma = 1.250000e-001
b = 1.000000e+000
Absolute Error Prediction = 1.394712e-003
Relative Error Prediction = 6.045705e-003
Tolerance Flag = 0

Walk clock time = 4.040000e+000
Press enter to exit the main program...
```

Conclusion

This software demonstrates the use of GPU acceleration for optimal parameter selection in a numerical Laplace transform inversion algorithm. The Weeks method is straightforward to parallelize and thus is a good candidate for GPU computations. The required fast Fourier transforms are also well implemented by NVIDIA on the GPU. More importantly, the algorithm actually performs on the tested problems despite the well known inherent ill-posedness of the numerical inverse Laplace transform.

The software is sufficient for illustration purposes but could be expanded and refined into a more user-friendly form. The codes are intended for adaption and use in other programs and tools. If they are used, a reference and e-mail to Acunum would greatly appreciated. The files are provided 'as is' with no guarantees under a standard BSD license.

References

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SIAM Journal on Scientific Computing
Volume 21 Issue 1, Aug.-Sept. 1999
http://dip.sun.ac.za/~weideman/research/weeks.html

[6] William T. Weeks
Numerical Inversion of Laplace Transforms Using Laguerre Functions
Journal of the ACM (JACM)
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Appendix – CUDA Setup

Two sets of code are supplied; one is for Windows with Visual Studio and the other is intended for Linux-like environments. The core source and header files are identical in both sets. The two cases reflects the different ways that the codes have been compiled. They were written on a ASUS N53S series laptop with Windows 7, an Intel i7 central processor, and an NVIDIA GeForce GT 540M graphics processor. This GPU has an NVIDIA compute capability of 2.1 and 96 cores.

Visual Studio

The codes have been compiled and tested with Visual Studio 2008. Setting up Visual Studio and CUDA to interface correctly on the laptop has been a nontrivial task. A useful reference is here:
http://www.codeproject.com/KB/GPU-Programming/visualstudioCUDA.aspx

A few more helpful comments are:

- Download and install Visual Studio 2008 (not 2010). Our own personal experience has shown that the 2008 works well with CUDA 3.2; see the blog:
  http://blog.cuvilib.com/2011/02/24/how-to-run-cuda-in-visual-studio-2010/

- Download and install the NVIDIA toolkit 3.2. A 4.0 release is available but was not used to develop this code.
  http://developer.nvidia.com/cuda-downloads

- Download and install the NVIDIA software development kit 3.2. It is also from:
  http://developer.nvidia.com/cuda-downloads

The included VS project has the CUDA configuration and properties set to work with a GPU with compute capability 2.1. It was however necessary to manually place some files and configure the visual studio project.

- add : C:\Program Files (x86)\Microsoft Visual Studio 9.0\VC\VCProjectDefaults\NvCudaDriverApi.v3.2

- add : C:\Program Files (x86)\Microsoft Visual Studio 9.0\VC\VCProjectDefaults\NvCudaRuntimeApi.v3.2

- Within the VS project add the build rules with: project -> Custom Build Rules-> CUDA Driver API Build Rule 3.2

- add manually : Tools->Options->Projects and Solutions->VC++ Project Settings ->
  C:\(the path)\NVIDIA_SOFTWARE\cudatoolkit_3.2_win_buildrules-patch

- add manually : Tools->Options->Projects and Solutions->VC++ Directories ->

1. Executable files: C:\Program Files\NVIDIA GPU Computing Toolkit\CUDA\v3.2\bin
2. Include files:
   a. C:\Program Files\NVIDIA GPU Computing Toolkit\CUDA\v3.2\include
   b. C:\ProgramData\NVIDIA Corporation\NVIDIA GPU Computing SDK 3.2\C\common\inc
3. Library files
   a. C:\Program Files\NVIDIA GPU Computing Toolkit\CUDA\v3.2\lib\Win32
   b. C:\ProgramData\NVIDIA Corporation\NVIDIA GPU Computing SDK 3.2\C\common\lib

Cygwin
To test compatibility, the codes were also compiled and run on the laptop using Cygwin
http://www.cygwin.com/

A MakeFile is provided for this purpose. It is simpler to use the MakeFile rather than Visual Studio. To create the executable, one simply uses on the command line the standard 'make'. 'make clean' is also provided to remove the object files. It is useful to 'make clean' when the 'UserFs.txt' file has been modified before one re-compiles for a new F(s). The MakeFile is currently setup to use the Windows 'cl' compiler.