Intel® MKL Data Fitting component. Overview

Intel Corporation

Agenda

- 1D interpolation problem statement
- Functional decomposition of the problem
- Application areas
- Data Fitting in Intel® MKL
- Data Fitting API and usage models
- Data Fitting performance

1D interpolation problem statement

For given table function {x(i), y(i)}, i=1,…,n where
x(i) - breakpoints in ascending order, y(i) – values

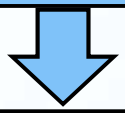
- Approximate function f(x): f(x(i))=y(i)
- Evaluate value f(t(j)) and derivative f’ (t(j))
  - Site t(j) is any real value [x(1),x(n)], j=1,…,m
- Evaluate integral of f(x) over interval [a(j),b(j))
  - Integration limits a(j) and b(j) belong to or are outside of interpolation interval [x(1),x(n)], j=1,…,m

1D interpolation problem statement

- **Splines – methodology for solution of interpolation problem**
  - Can be preferable vs polynomial interpolation
    - Runge's phenomenon
      - Interpolation error for g(x)=1/(1+25x^2) increases with order of the polynomial
- **Spline – piece-wise polynomial function**
  - g(x) := Pj(x), x belongs to [x(j), x(j+1))
    - Pj(x) -polynomial of degree k on the interval [x(j), x(j+1))
  - Spline - smooth up to order q at x(j) if values of derivatives up to order q for P(j-1) and Pj at x(j) exist and equal

Functional decomposition of the problem

Construct spline of given order
for n break points x(i)



Compute value of spline and/or its derivative
at M interpolation sites t(j), m>>n

Find interval [x(i), x(i+1)) containing t(j)

Compute value of Pi polynomial at t(j)

Integration has similar computational flow
Search – key building block

Application areas

- **Data analysis and analytics**
  - Approximation of statistical estimates like histogram
- **Manufacturing**
  - Geometrical modeling
  - *"B-spline recurrence relations … were used at Boeing, …, five hundred million times a day"* Carl de Boor, On Wings of Splines Newsletter of Institute for Mathematical Sciences, ISSUE 5 2004
- **Energy**
  - Surface approximation
- **ISV**
  - SW libraries

Data Fitting in Intel® MKL

- **Intel® MKL Data Fitting – SW solution for**
  - Spline construction
  - Spline based interpolation and computation of derivatives
  - Spline based integration
  - Cell Search

Data Fitting in Intel® MKL

- **Components of Intel® MKL Data Fitting**

Spline construction

Spline	Spline type	Boundary conditions	Internal conditions
Linear		Not-a-knot	1st derivative
Quadratic	Default, Subbotin	Free-end	2nd derivative
Cubic	Default, Natural, Hermite, Bessel, Akima	1st derivative at the left/right endpoint	Knot array
Look-up		2nd derivative at the left/right endpoint	
Stepwise constant	Continuous-right, Continuous-left	Periodic	
User-defined		Function value at mid point of first cell	

Rich collection of splines that support different boundary or/and internal conditions

Data Fitting in Intel® MKL

- **Components of Intel® MKL Data Fitting**

Interpolation/extrapolation/integration

Feature	Comment

Computation of value, derivative of arbitrary order	• Support of a-priori information about structure of partition, and/or interpolation sites
	• In addition to default spline based interpolation library supports user-defined functions to
	  • re-define default spline based computations on interpolation or/and extrapolation intervals
	  • re-define cell search functions
	• Option to get results of cell search simultaneously with interpolation
	• User defined threading-friendly API

Computation of integrals	• Support of a-priori info about structure of partition, and/or integration limits
	• In addition to default spline based interpolation library supports user-defined functions to
	  • re-define default integration on interpolation or/and extrapolation intervals
	  • re-define cell search functions
	• User defined threading-friendly API

Flexibility in support of various usage models for spline based computations

Data Fitting in Intel® MKL

- **Components of Intel® MKL Data Fitting**

Search

Feature	Comment
Computation of cell indices containing given sites	• Support of a-priori information about structure of partition, and/or interpolation sites • In addition to default cell search computation library supports user-defined function to • re-define cell search functions • User defined threading-friendly API

Flexibility in support of various usage models for cell search

Data Fitting API and usage models

Step	Code example	Comment
Create a task	`status = dfdNewTask1D( &task, nx, x, xhint, ny, y, yhint );`	You can call the Data Fitting function several times to create multiple tasks
Modify the task parameters.	`status = dfdEditPPSpline1D( task, s_order, c_type, bc_type, bc, ic_type, ic, scoeff, scoeffhint );`	
Perform Data Fitting spline-based computations	`status = dfdInterpolate1D(task, estimate, method, nsite, site, sitehint, ndorder, dorder, datahint, r, rhint, cell );`	You may reiterate steps 2-3 as needed
Destroy the task or tasks	`status = dfDeleteTask( &task );`	

API and usage model similar to that in Vector Statistical component, Fourier Transforms in Intel® MKL

Data Fitting API and usage models

Cubic Spline-Based Interpolation

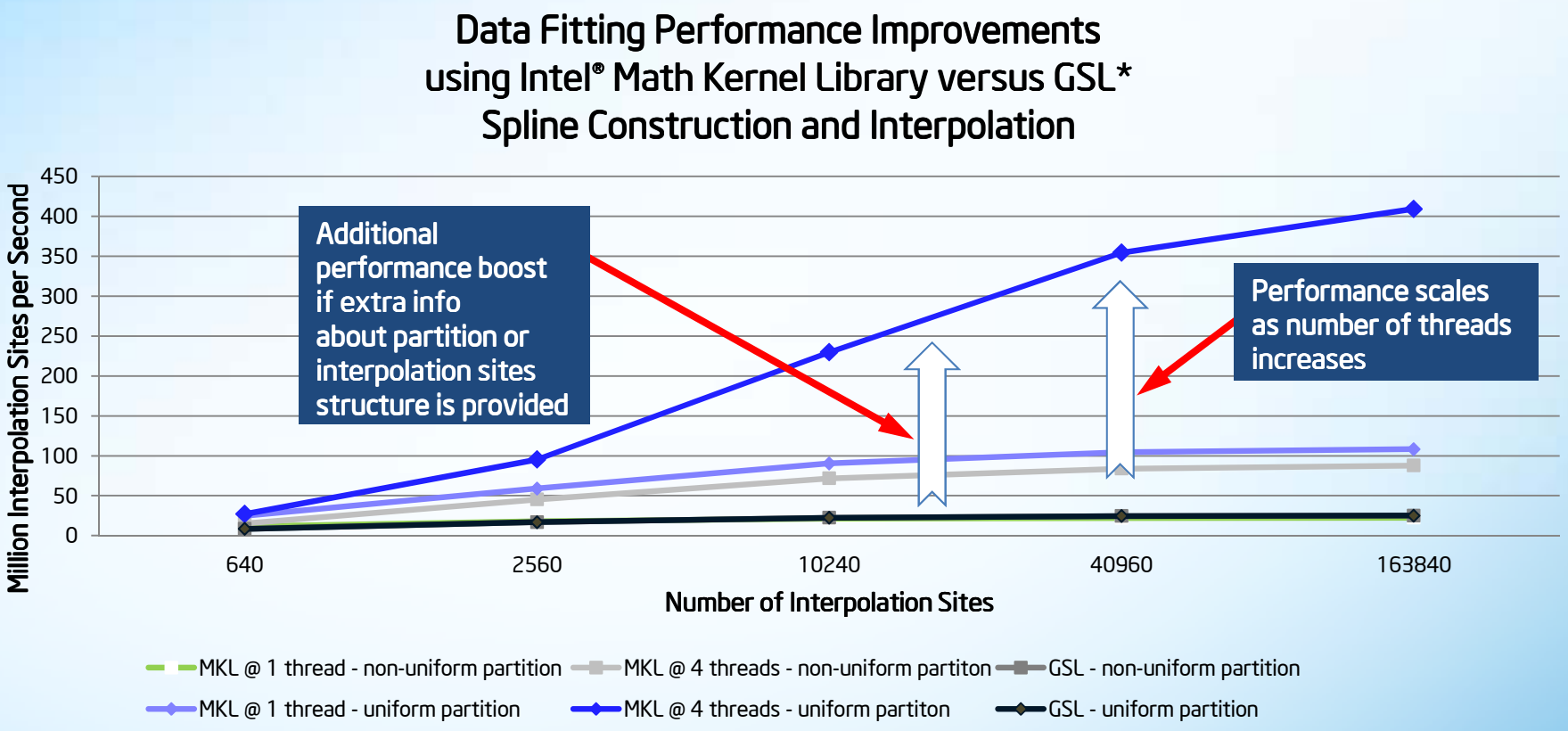
```
#include "mkl.h"

int main(){
    /* Initialize the partition and set their values */
    nx = N;
    xhint = DF_NON_UNIFORM_PARTITION /* The partition is non-uniform. */
    /* Initialize the function and set their values */
    ny = 1; /* The function is scalar. */
    yhint = DF_NO_HINT; /* No additional information about the function is provided. */
    /* Create a Data Fitting task */
    status = dfdNewTask1D( &task, nx, x, xhint, ny, y, yhint );

    /* Initialize spline parameters */
    s_order = DF_PP_CUBIC; /* Spline is of the fourth order (cubic spline). */
    s_type = DF_PP_BESSEL; /* Spline is of the Bessel cubic type. */

    ic_type = DF_NO_IC; ic = NULL; /* Define internal conditions for cubic spline construction (none in this example) */
    bc_type = DF_BC_NOT_A_KNOT; bc = NULL; /* Use not-a-knot boundary conditions */
    scoeffhint = DF_NO_HINT; /* No additional information about the spline. */

    /* Set spline parameters in the Data Fitting task */
    status = dfdEditPPSpline1D( task, s_order, s_type, bc_type, bc, ic_type, ic, scoeff, scoeffhint );
    /* Construct a cubic Bessel spline: Pi(x) = c1,i + c2,i(x - xi) + c3,i(x - xi)^2 + c4,i(x - xi)^3; the library packs spline
        coefficients to scoeff: scoeff[4*i+0] = c1,i, scoef[4*i+1] = c2,i,  scoeff[4*i+2] = c3,i, scoef[4*i+1] = c4,i */
    status = dfdConstruct1D( task, DF_PP_SPLINE, DF_METHOD_STD );

    /* Initialize interpolation parameters and set site values */
    nsite = NSITE;
    sitehint = DF_NON_UNIFORM_PARTITION; /* Partition of sites is non-uniform */
    ndorder = 1; dorder = 1; /* Request to compute spline values */
    datahint = DF_NO_APRIORI_INFO;  /* No additional information about breakpoints or sites is provided. */
    rhint = DF_MATRIX_STORAGE_ROWS; /* The library packs interpolation results in row-major format. */
    cell = NULL; /* Cell indices are not required. */
    /* Compute the sline values at the points site(i), i=0,..., nsite-1 and place the results to array r */
    status = dfdInterpolate1D(task, DF_INTERP, DF_METHOD_STD,nsite, site, sitehint, ndorder, &dorder, datahint, r, rhint, cell );

    /* De-allocate Data Fitting task resources */
    status = dfDeleteTask( &task );
    return 0;
}
```

Data Fitting API and usage models

Cell Search

```
#include "mkl.h"

int main(){
   /* Initialize a uniform partition */
   nx = N;
   /* Set values of partition x: for uniform partition, provide end-points of the interpolation interval [-1.0,1.0] */
   x[0] = -1.0f; x[1] = 1.0f;
   xhint = DF_UNIFORM_PARTITION; /* Partition is uniform */

   /* Initialize function parameters; in cell search, function values are not necessary and are set to zero/NULL values
*/
   ny = 0;
   y = NULL;
   yhint = DF_NO_HINT;

   /* Create a Data Fitting task */
   status = dfdNewTask1D( &task, nx, x, xhint, ny, y, yhint );
   ...
   /* Initialize interpolation (cell search) parameters */
   nsite = NSITE;
   /* Set sites in the ascending order */
   ...
   sitehint = DF_SORTED_DATA; /* Sites are provided in the ascending order. */
   datahint = DF_NO_APRIORI_INFO; /* No additional information about breakpoints/sites is provided.*/

   /* Compute indices of the cells that contain interpolation sites. The library places the index of the cell containing
      site(i) to the cell(i), i=0,...,nsite-1 */
   status = dfSearchCell1D( task, DF_METHOD_STD, nsite, site, sitehint, datahint, cell );

   /* Process cell indices */
   status = dfDeleteTask( &task );
   return 0;
}
```

Data Fitting performance



Construction of natural cubic spline with free end boundary conditions for function defined on uniform and non-uniform partitions. Partition size is 1280. Spline-based values and first derivatives are computed.

Configuration Info - Versions: Intel® Math Kernel Library (Intel® MKL) 10.3.8 GSL 1.15; Hardware: Intel® Core® i7-2600 Processor, 3.40Ghz, 8 MB L2 cache, 4 GB Memory; Operating System: Fedora 14 x86_64; Benchmark Source: Intel Corporation.

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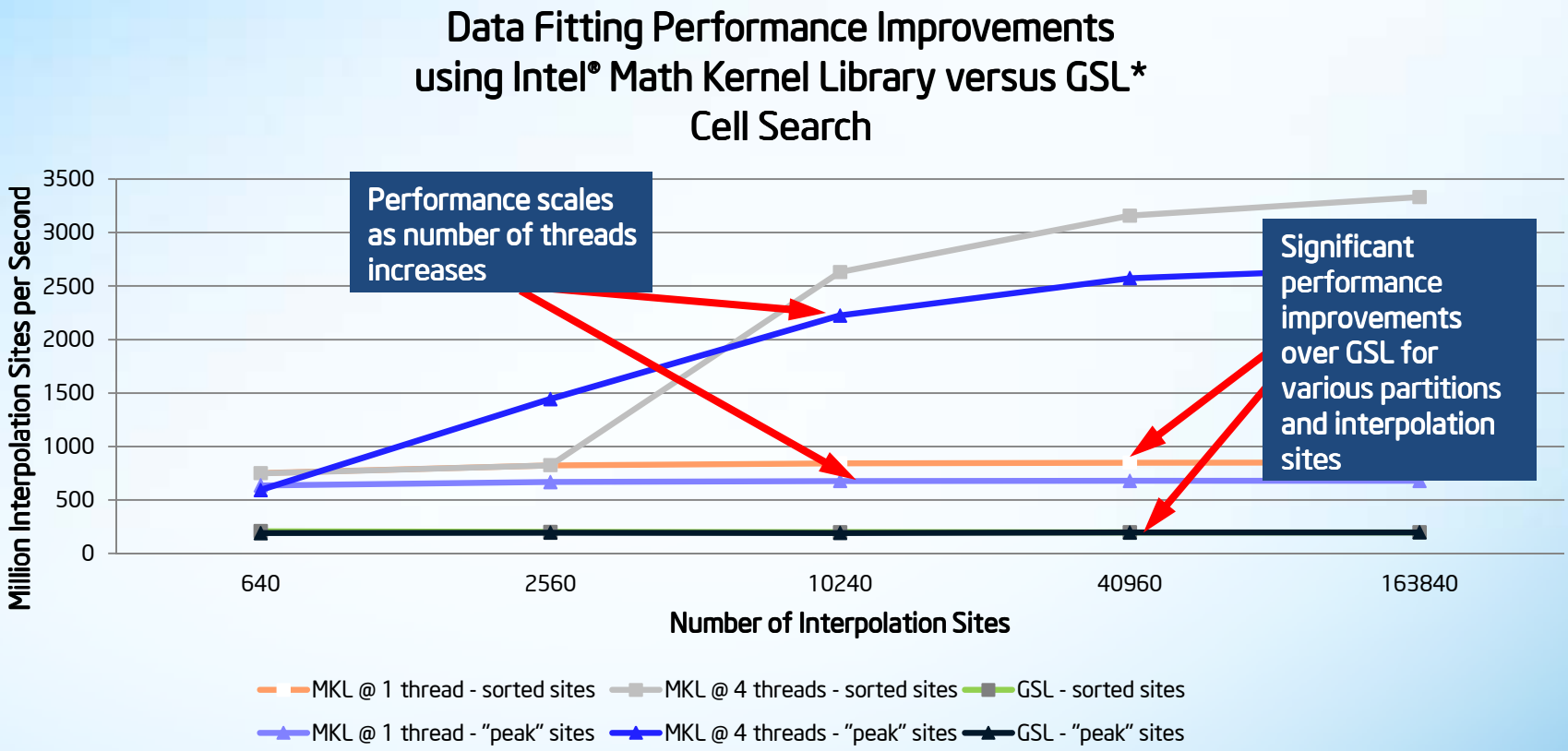
Data Fitting performance



Performing cells search on non-uniform partition. Partition size is 1280.
Sorted sites - interpolation sites are sorted ; "peak" sites - distribution of interpolation sites has a clear peak.

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