High-Performance Vectorization on GPU Cluster by MVAPICH2

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Introduction
Accelerator

	Nvidia Kepler K20X	Intel Xeon Phi 7120
Launch Date	November 2012	Q2 2013
Processor	14 Streaming Multiprocessors	61 Pentium x86 cores
Per-processor Concurrency	192 CUDA cores (SIMT)	4 hyperthreads ×8(512 bit)× SIMD units
Total Nominal Concurrency	2688 (14×192)	1952 (61×4×8)
Acceleration Techniques	Vectorization, Shared memory, OpenACC	Vectorization

Introduction

Vectorization: a data-level parallelism, vectorization is the process of converting an algorithm from a scalar implementation, which does an operation one pair of operands a time, to a vector process, where a single instruction can refer to a vector (series of adjacent values.)

Mark Sabahi, et al., A Guidance to Vectorization with Intel C++ Compilers, P. 1, Intel Corporation.

Introduction
Vectorization

- **loop vectorization: independent loop,** loop with if conditions, *etc*.;
- matrix tile: element tile, row/column tile, matrix tile, *etc*.;
- index operations: idx2val, val2idx, find, fetch/write by index, *etc*.;
- element-wise binary operation;
- logical operation: all, any, logical, *etc*.;
- *etc*.;

Application: all fields

- high-performance optimizer;
- high-performance integration;
- high-performance sampler;
- high-performance tri-diagonal solver, halo exchange;
- high-dimensional look-up table;
- *etc*.;

- Building blocks for high-level fields such as machine learning and artificial intelligence, computer graphics, computer vision, simulation, *etc*.;
- Usually defined on single GPU, research needed for multi-GPU and GPU cluster;

Introduction

Vectorization: *for-loop*

for i = 1:I
operation (i);
end

operation(I)

	Computational Cost	Memory Cost
for-loop	I	1
vectorization	1	I

SIMD

Introduction
Vectorization: *2-nested for-loop*

for $i_1 = 1{:}I_1$
for $i_2 = 1{:}I_2$
operation (i_1, i_2);
end
end

operation$(I_1 * I_2)$

	Computational Cost	Memory Cost
for-loop	$I_1 * I_2$	1
vectorization	1	$I_1 * I_2$

vectorization of 2-nested loop applications: find (for data compression), bin locating, *etc.*;

Introduction

Vectorization: *k-nested for-loop*

for $i_1 = 1:I_1$
  for $i_2 = 1:I_2$
    ●●●
    for $i_k = 1:I_k$
      operation $(i_1, i_2, \cdots i_k)$;
    end
    ●●●
  end
end

operation$(I_1 * I_2 \cdots I_k)$

	Computational Cost	Memory Cost
for-loop	$I_1 * I_2 \cdots I_k$	1
vectorization	1	$I_1 * I_2 \cdots I_k$

vectorization of *k*-nested loop applications: building high-dimensional look-up table

Introduction

Vectorization: *k-nested for-loop*

- **For nested for-loop, memory cost increases Exponentially!**
- **For applications such as high-dimensional approximation, large $I_1 * I_2 \cdots I_k$ is needed for high accuracy;**
- **For applications such as two-dimensional approximation, even two-dimensional $I_1 * I_2$ is too big to fit in GPU's global memory;**
- **Best performance of kernel execution comes from suitable setting the number of blocks and the number of threads per block, operation on full memory usually leads to bad performance;**

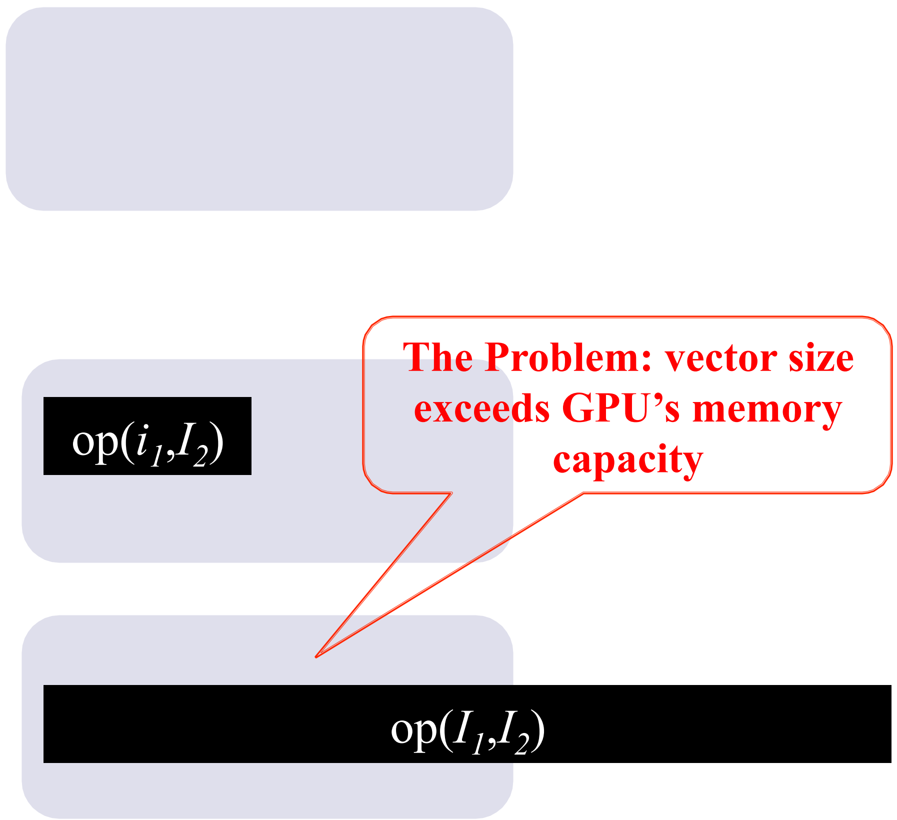
Introduction

GPU-cluster Vectorization: *2-nested loop*

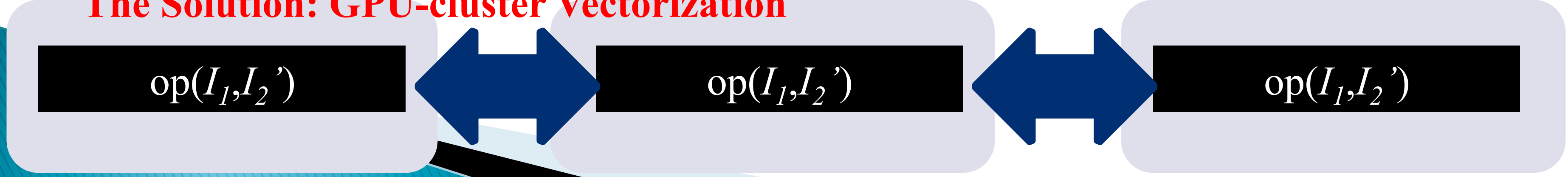
for $i_1 = 1{:}I_1$
  for $i_2 = 1{:}I_2$
    operation (i_1,i_2);
  end
end

for $i_2 = 1{:}I_2$
  operation (i_1,I_2);
end

operation (I_1,I_2);



The Solution: GPU-cluster Vectorization



Introduction
GPU-cluster Vectorization: *2-nested loop*

- Step 1: In master GPU, separation of the array (I_1, I_2);
- Step 2: Send the separated array (I_1, I_2') by MPI_SCATTER;
- Step 3: Vectorized operation op (I_1, I_2') in each GPU;
- Step 4: Collect the partial results to master GPU by MPI_GATHER;
- Step 5: In master GPU, assembly the partial results back to the array (I_1, I_2);

- **In GPU-cluster vectorization, Step 1, Step 3 and Step 5 is done in single GPU;**
- **In GPU-cluster vectorization, the size of (I_1, I_2') usually hundreds of kb, since the number of GPU is limited;**
- **The performance of GPU-cluster vectorization is decided by the two collective communications: MPI_SCATTER and MPI_GATHER, especially while GPU-cluster vectorization locates in iteration or time step;**
- **MVAPICH2;**
- **Vectorization of *k*-nested loop is more complicated in communication;**

Methods

High-performance Optimizer: an example of vectorization on GPU Cluster by MVAPICH2

Bin Locating

↓

Iterative Discrete Approximation

↓

High-performance Optimizer

Methods
Bin Locating

- **Bin Locating:** Two arrays *S* and *D*: the array *S* is a sequence, the array *D* is data. For a element d_i in *D*, find the range $s_i <= d_j < s_{i+1}$ in array *S*;
- **Implementation:** comparing element d_i in *D* against the sequence *S* one by one;

Methods

Bin Locating

- 2-nested for-loop: inner loop and outer loop. Computational Cost: I × J; memory cost: 1;

```
for i = 1:I
    for j = 1:J
        if ( s(j) <= d(i) & d(j) < s(i+1) )
        bin(i) = j;
        break;
    end
end
```

- Vectorization of inner-loop. Computational Cost: I ; memory cost: 1;

This element is tiled to array with size J

```
for i = 1:I
        bin = sum( d(i) – S);
end
```

Methods
Bin Locating

- Vectorization of outer-loop. Computational Cost: 1; memory cost: $I \times J$;

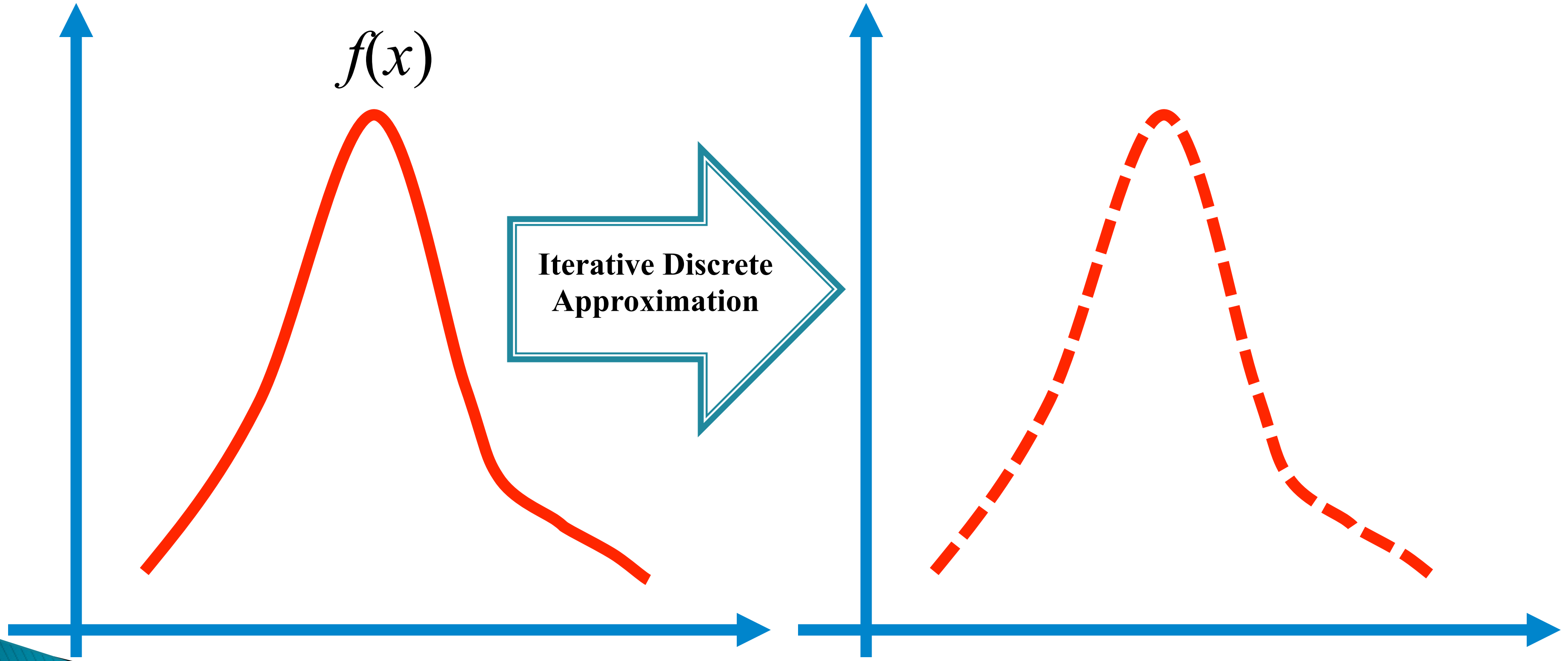
bin = ***sumrow*** **(tile(*D*, *J'*) − tile(*S*, *I*));**

- Splitting the array tile(D, J') and tile(S, I) across multi-GPUs by MPI_Scatter;
- The computation of comparison is done in each GPU;
- Reduction *sumrow* is implemented by CUDA thrust;
- Partial results are gathered by MPI_Gather;
- The Master-Slave Paradigm: master node and master GPU;

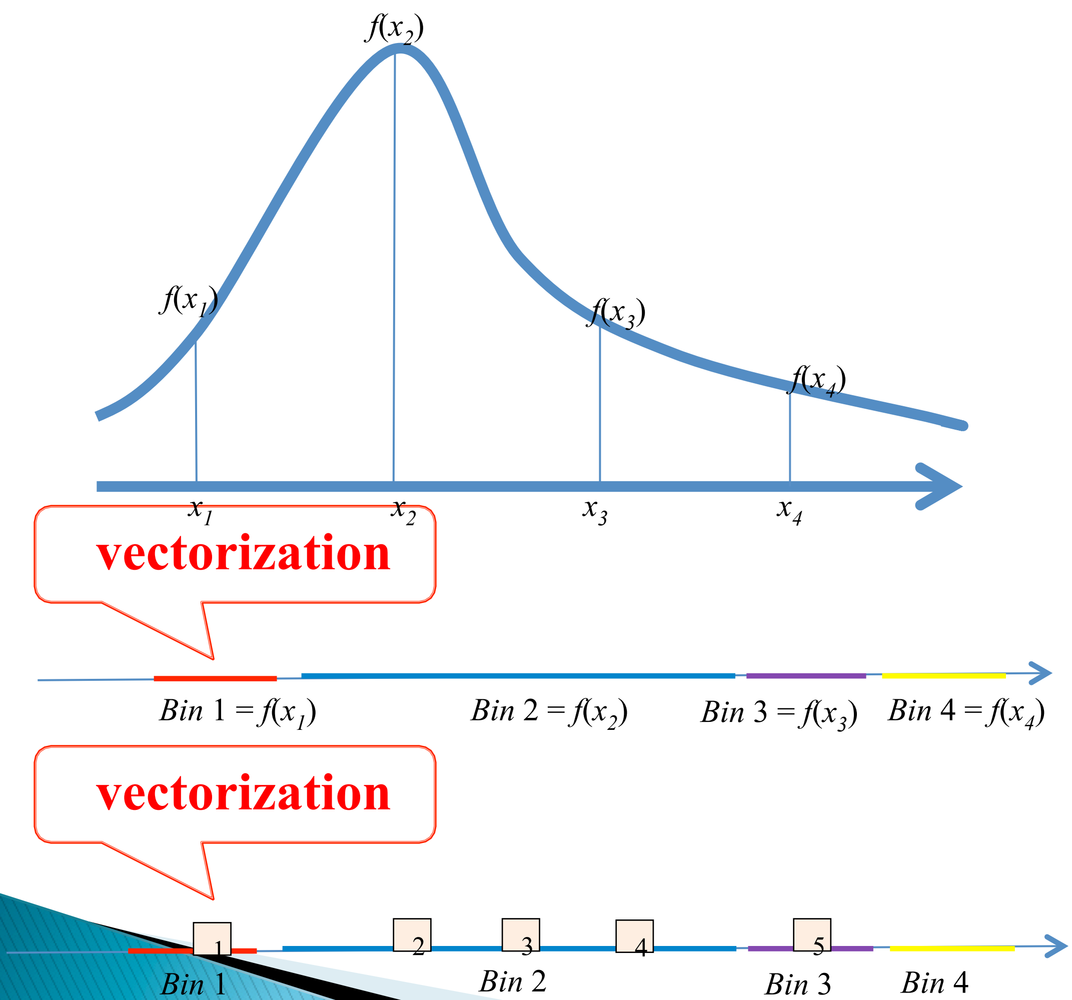
Method
Iterative Discrete Approximation

- Iterative Discrete Approximation approximates complicated continuous distributions by discrete random numbers;
- Large portion of computation of Iterative Discrete Approximation is spent on bin locating;

Methods
Iterative Discrete Approximation



Methods
Iterative Discrete Approximation

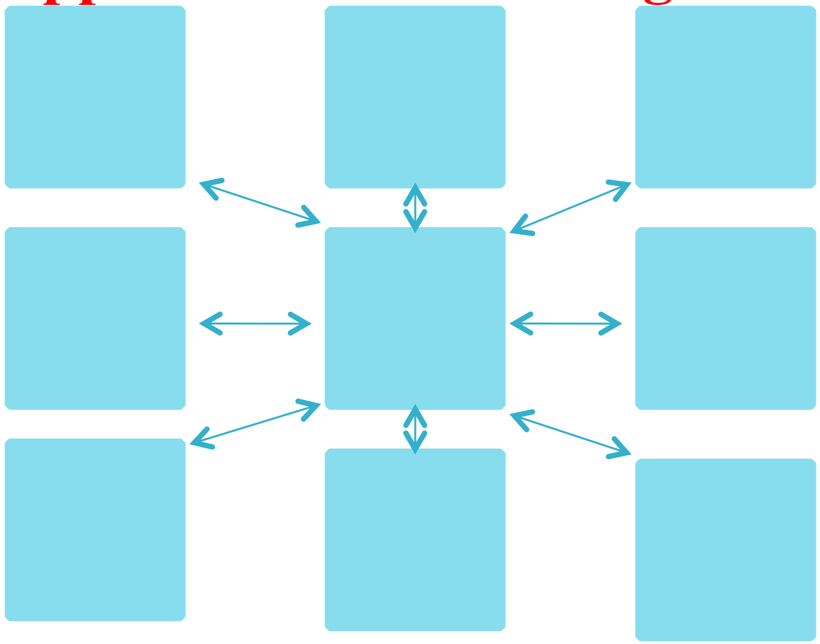


- Generate random numbers of uniform distribution;
- Estimation the shape of the function $f(x)$;
- Take advantage of the estimated shape, discretely approximate the function $f(x)$ by iterations;
- Implemented by GPU cluster;

Methods

High-Performance Optimizer

For large-scale and complicated search space, single Iterative Discrete Approximation is efficient, parallelization techniques are applied to make multiple Iterative Discrete Approximation work together.



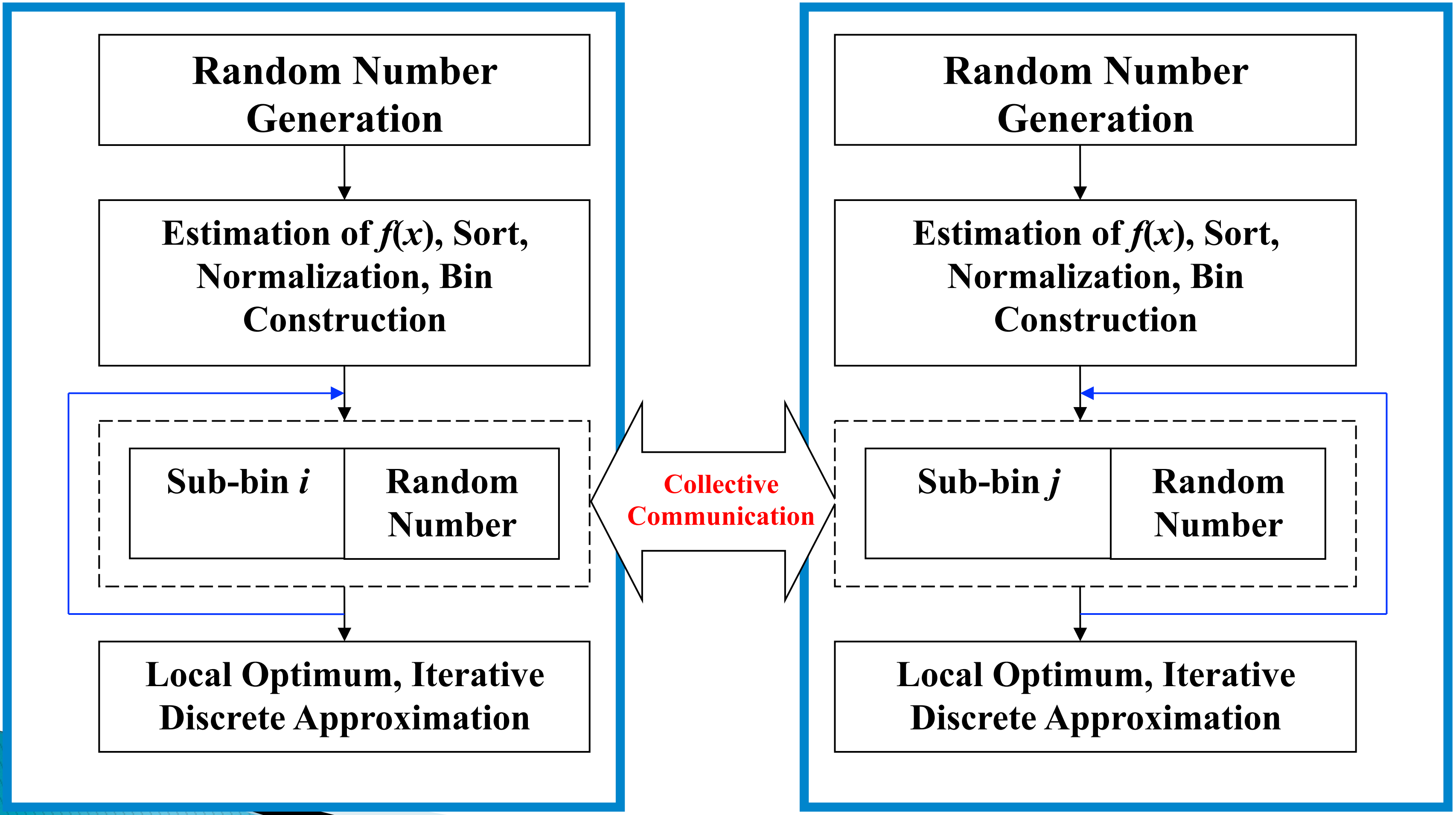
Domain Decomposition of Search Space: understanding vectorized bin locating in the language of optimization

Methods

High-Performance Optimizer

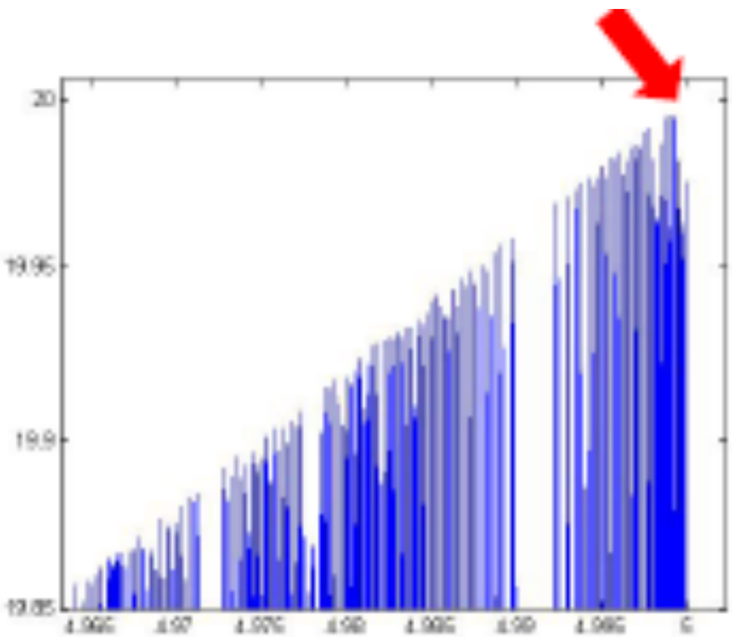
- The search space is equally separated into multiple sub-space, and sent to each GPU by MPI_SCATTER;
- The search space keeps changing in each iteration;
- Each GPU is responsible for a sub-space;
- Each GPU generates local optimum;
- Local optima is collected by MPI_ALLREDUCE to calculate global optimum for next iteration;

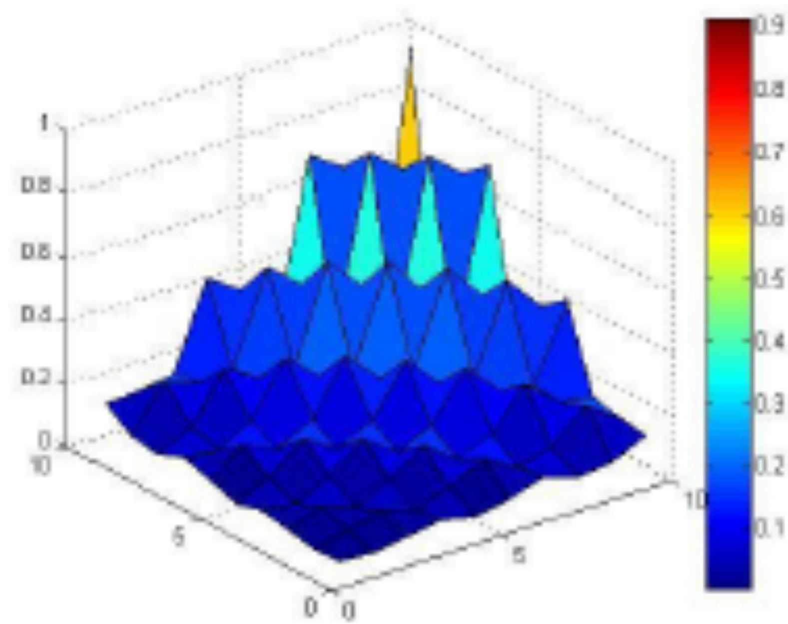
Methods
High-Performance Optimizer



Computational Results

The problem: Finding the maximum peak from all peaks

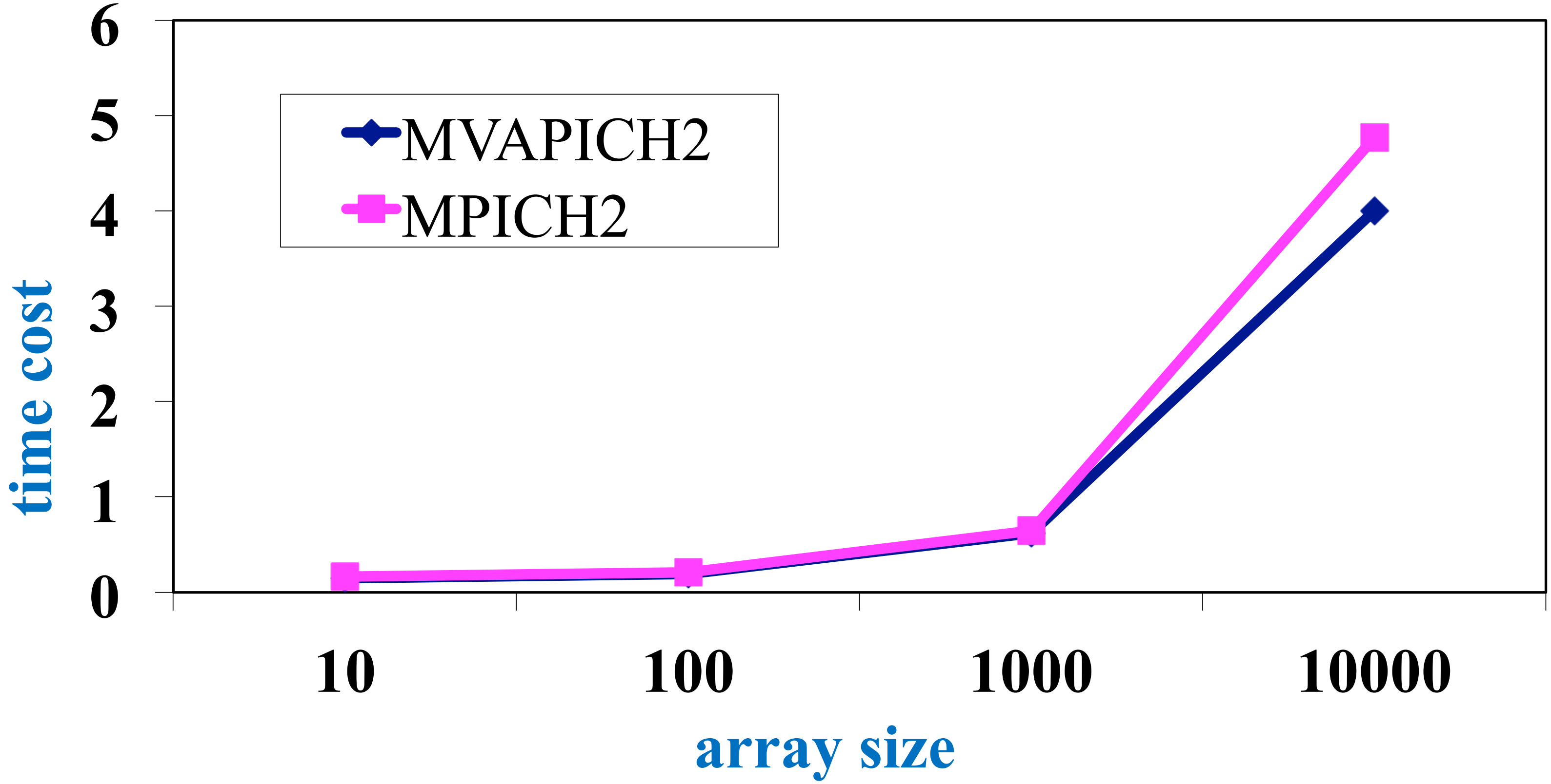




$$\max_{x} f(x) = a \times x \times abs(\sin(bx)^{c})$$

$$f(x,y) = abs\left(\frac{x}{a} \times \frac{y}{b} \times \sin(x+y)\right)$$

Computational Results

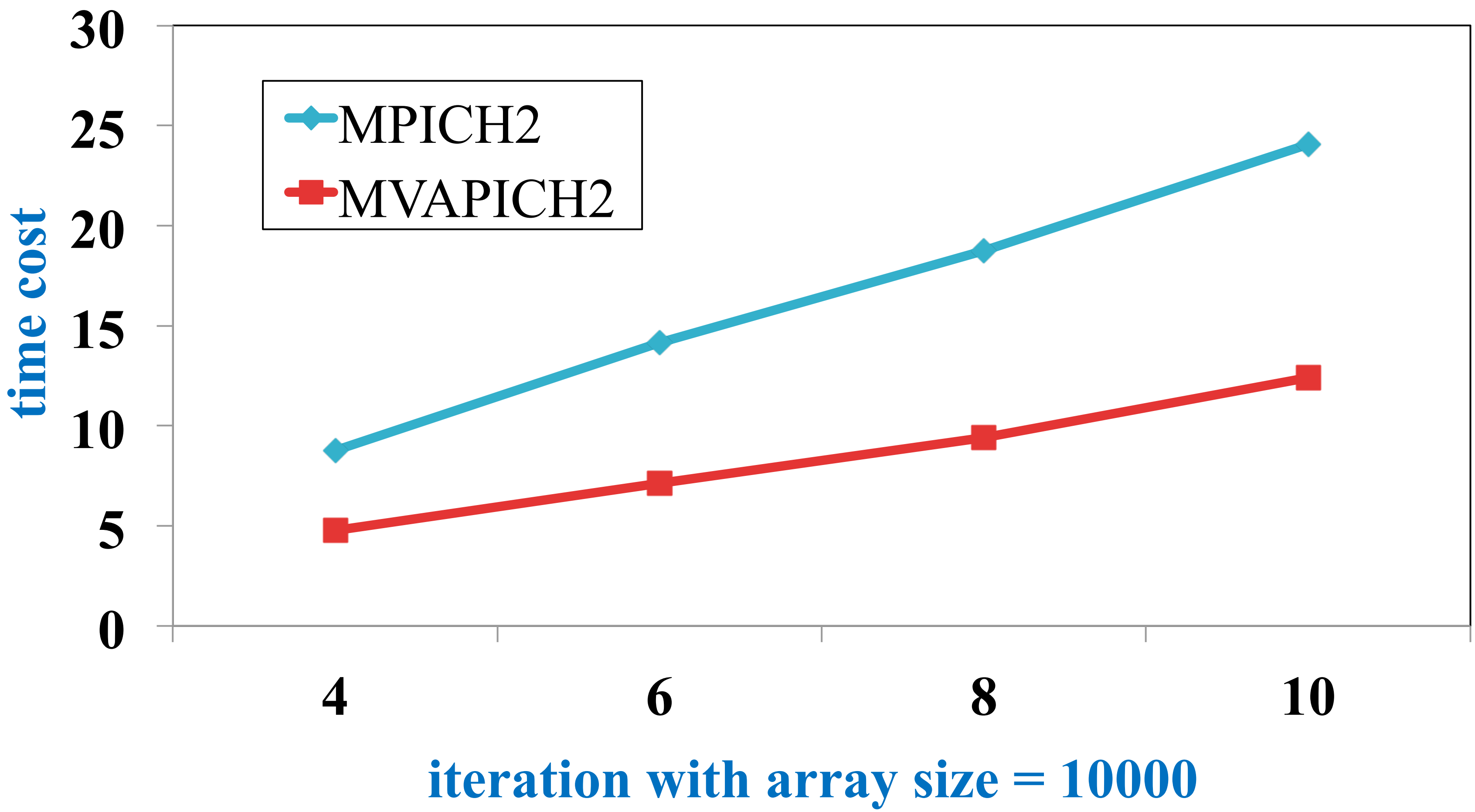


array size: the size of multiple arrays, not completely equal to message size

Time Cost of the Fourth Iteration by
MVAPICH2 *v.s.* MPICH2

OSC Oakley cluster: 16 NVIDIA Tesla M2070, Mellanox IB QDR MT26428 Adapter

Computational Results



Time Cost along with Iterations by
MVAPICH2 *v.s.* MPICH2

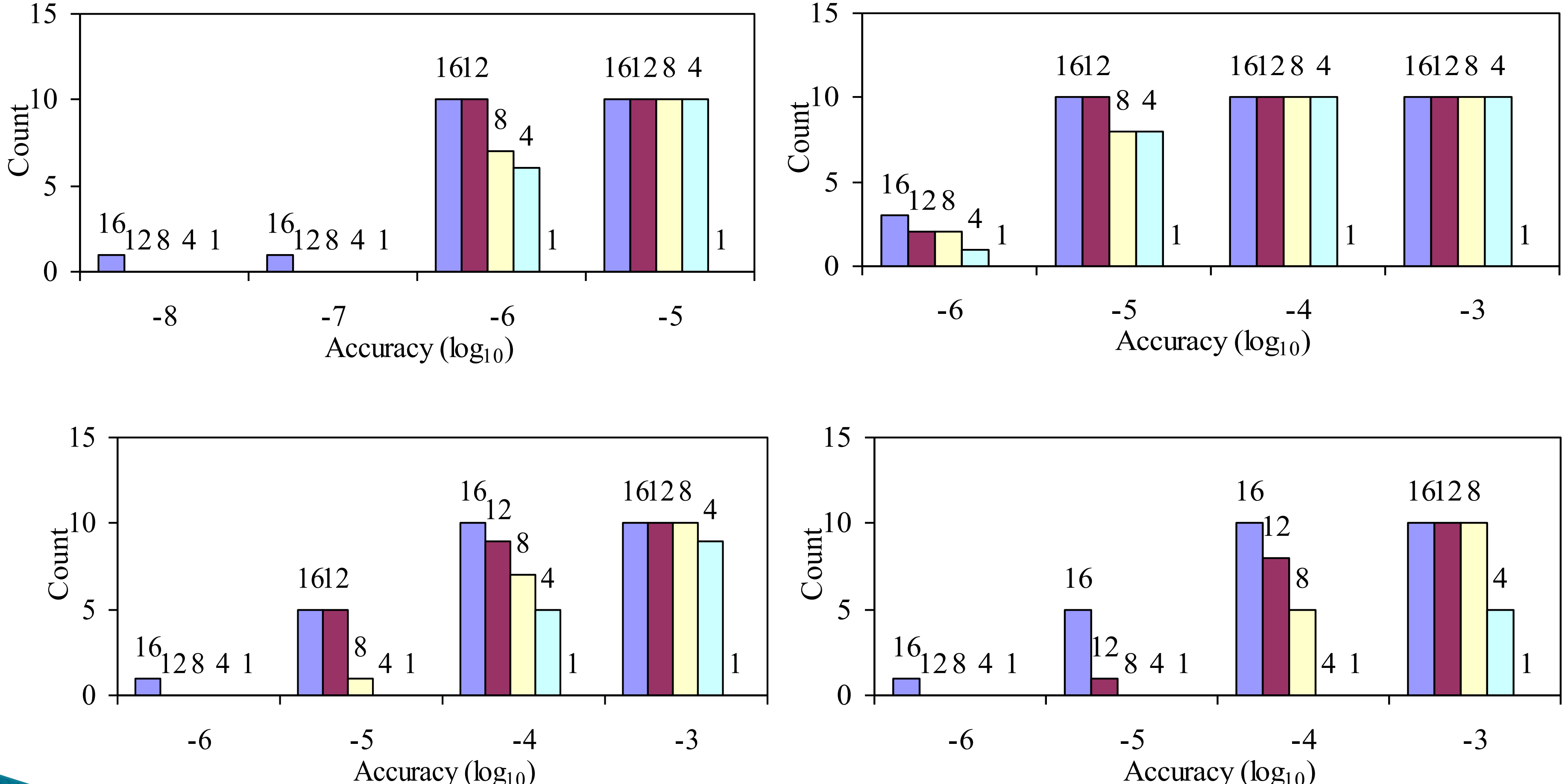
OSC Oakley cluster: 16 NVIDIA Tesla M2070, Mellanox IB QDR MT26428 Adapter

Computational Results

	Dimension	Numbers of Peaks	Accuracy
Single GPU	1D	232	10^{-8}
Multi-GPU	1D	241,717	10^{-8}
GPU-Cluster	2D	317,038	10^{-6}

The Performance of Optimizer on GPU Clusters by MVAPICH2

Computational Results



Accuracy along with Number of GPUs (i) left up array size = 10000 (ii) right up array size = 1000 (iii) left down array size = 100 (iv) right down array size = 10

Conclusions

- MVAPICH2 significantly improves the performance of vectorization, leading to a high-efficiency applications such as optimizer;
- MVAPICH2 based GPU cluster is the platform to improve parallel programming techniques such as vectorization;
- More research of MVAPICH2 should be applied to more vectorization techniques;

Thanks !