

ReproBLAS: Reproducible BLAS

<http://bebop.cs.berkeley.edu/reproblas/>

James Demmel, **Nguyen Hong Diep**

SC'13 - Denver, CO

Nov 22, 2013

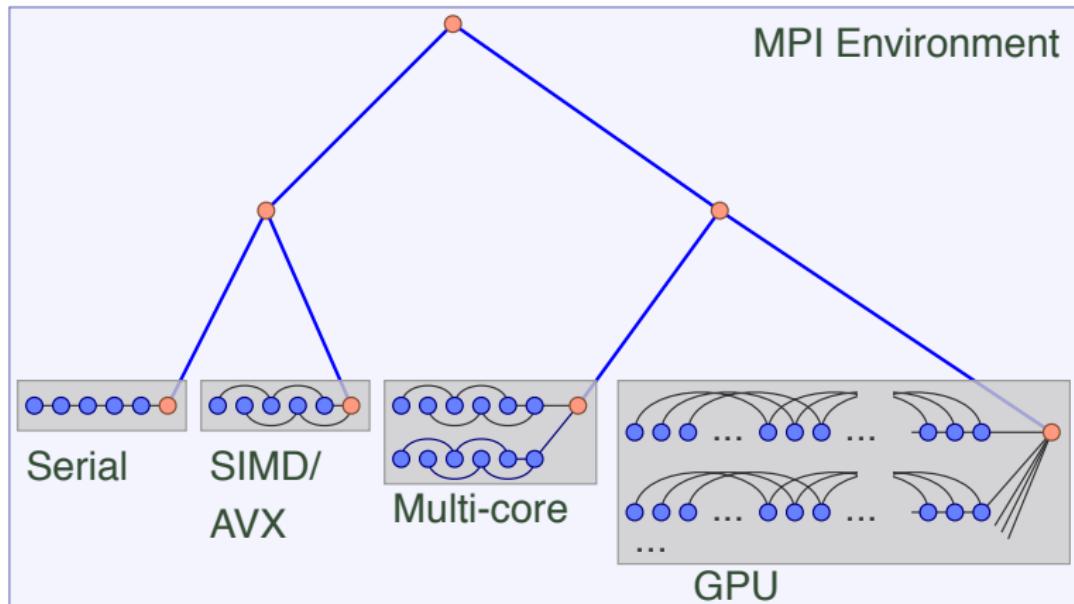
Reproducibility

Reproducibility: obtaining bit-wise identical results from different runs of the program on the same input data, regardless of different available resources.

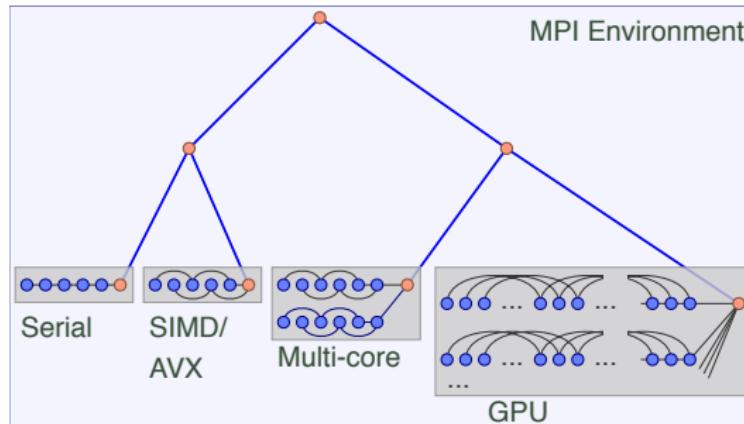
Cause of nonreproducibility: *not* by roundoff error but by the *non-determinism* of accumulative roundoff error.

Due to the *non-associativity* of floating point addition, accumulative roundoff errors depend on the order of evaluation, and therefore depend on available computing resources.

Sources of non-reproducibility

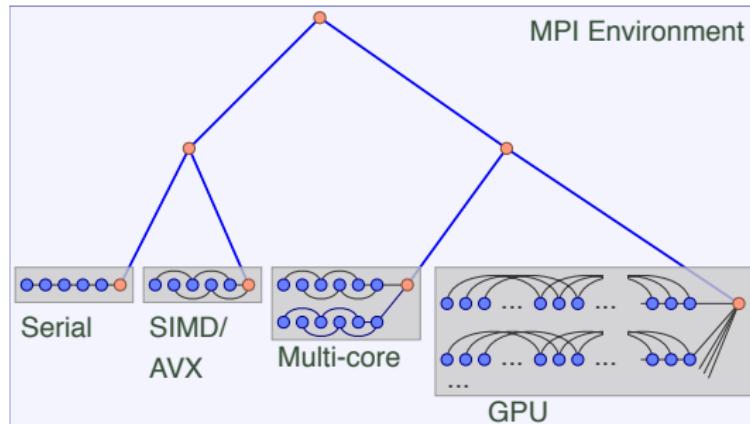


Sources of non-reproducibility



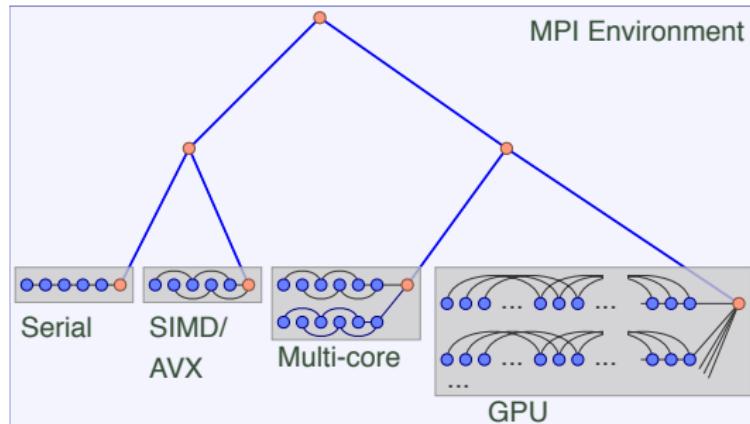
► number of MPI nodes

Sources of non-reproducibility



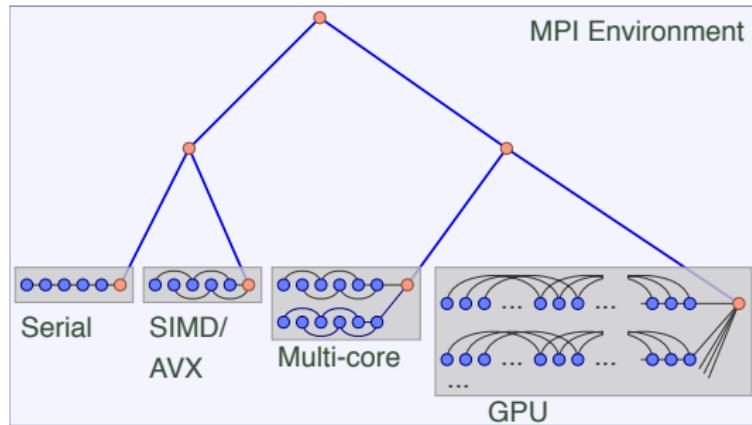
- ▶ number of MPI nodes
- ▶ MPI reduction tree shape

Sources of non-reproducibility



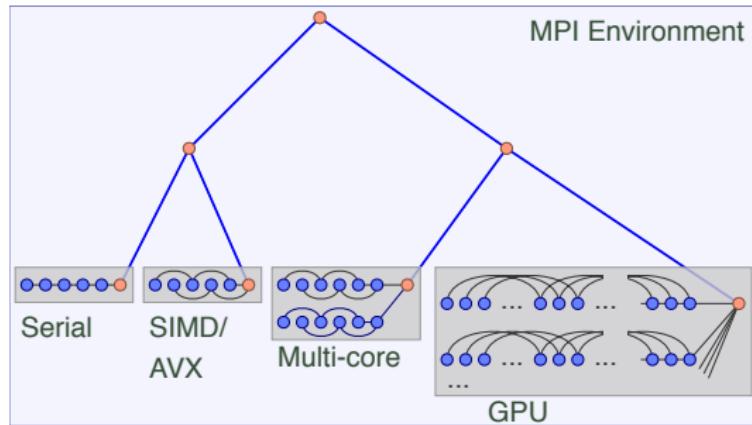
- ▶ number of MPI nodes
- ▶ MPI reduction tree shape
- ▶ number of cores per node

Sources of non-reproducibility



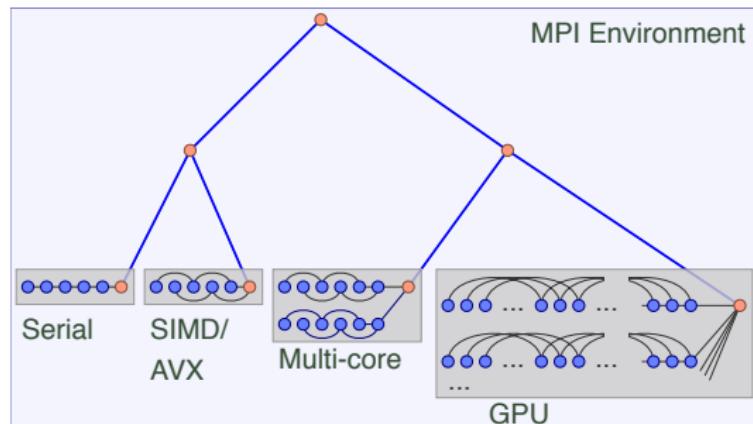
- ▶ number of MPI nodes
- ▶ MPI reduction tree shape
- ▶ number of cores per node
- ▶ data path (1,2,4,...)

Sources of non-reproducibility



- ▶ number of MPI nodes
- ▶ MPI reduction tree shape
- ▶ number of cores per node
- ▶ data path (1,2,4,...)
- ▶ data ordering

Sources of non-reproducibility

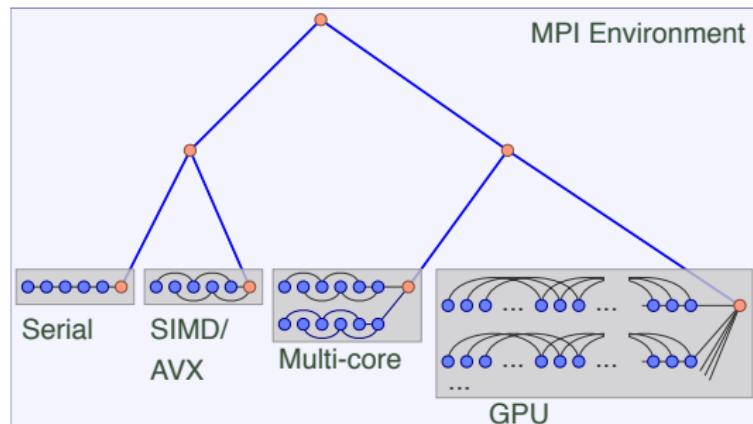


- ▶ number of MPI nodes
- ▶ MPI reduction tree shape
- ▶ number of cores per node
- ▶ **data path (1,2,4,...)**
- ▶ data ordering

Related work:

- ▶ Intel MKL 11.0 with CNR: reproducible with fixed number of processors, ~~and fixed data alignment~~,

Sources of non-reproducibility



- ▶ number of MPI nodes
- ▶ MPI reduction tree shape
- ▶ number of cores per node
- ▶ data path (1,2,4,...)
- ▶ data ordering

Related work:

- ▶ Intel MKL 11.0 with CNR: reproducible with fixed number of processors, and fixed data alignment,
- ▶ Hardware (NIC) for reproducible reduction operator.

Proposed solution

Goal: obtaining *deterministic* roundoff errors.

Exact arithmetic: unacceptably expensive in both long-word arithmetics and communication

Fixed point arithmetic:

- ▶ limited in exponent range
- ▶ limited in value range

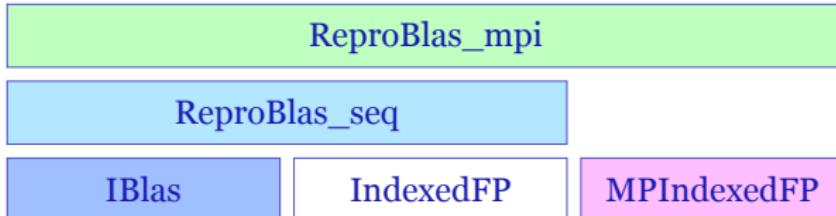
Indexed floating point: ¹

- ▶ Use floating point numbers to represent extended-precision fixed point,
- ▶ Exponent is of format $i \cdot W$ and is adjusted (on-line) according to the maximum absolute value of input,
- ▶ Can add up to 2^{60} floating point numbers,
- ▶ No extra reduction required for distributed environment,

¹J. Demmel and H. D. Nguyen, *Fast Reproducible Floating-Point Summation*, ARITH21, Austin, Texas, April 7–10, 2013

ReproBLAS: Reproducible Basic Linear Algebra Subprograms

URL: <http://bebop.cs.berkeley.edu/reproblas>



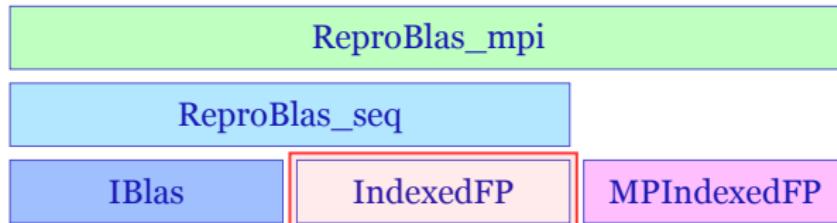
Features:

- ▶ Reproducibility,
- ▶ Accuracy: no severe accuracy loss,
- ▶ Reasonable arithmetic cost,
- ▶ Minimize communication: only one reduction per sum.

Requirements: **ROUND-TO-NEAREST** and *no overflow*

ReproBLAS: Reproducible Basic Linear Algebra Subprograms

URL: <http://bebop.cs.berkeley.edu/reproblas>

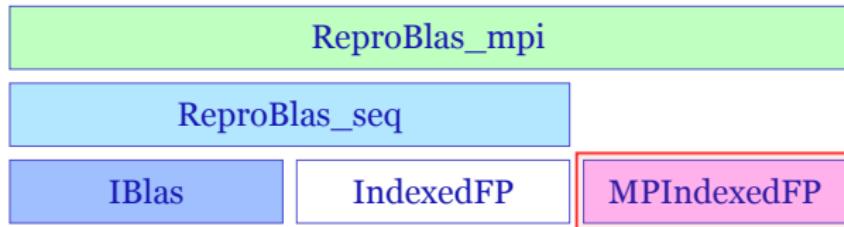


IndexedFP implement arithmetics for Indexed Floating Point:

- ▶ Data types: `Idouble`, `Ifloat`, `dIcomplex`, `sIcomplex`
- ▶ Conversion to: `dconv2I`, `sconv2I`, `zconv2I`, `cconv2I`
- ▶ Conversion from: `Iconv2d`, `Iconv2f`, `Iconv2z`, `Iconv2c`
- ▶ Addition: `dIAAdd`, `sIAAdd`, `zIAAdd`, `cIAAdd`
- ▶ Cross-type operations: `dIAAddd`, `sIAAddf`, `zIAAddz`, `cIAAddc`

ReproBLAS: Reproducible Basic Linear Algebra Subprograms

URL: <http://bebop.cs.berkeley.edu/reproblas>

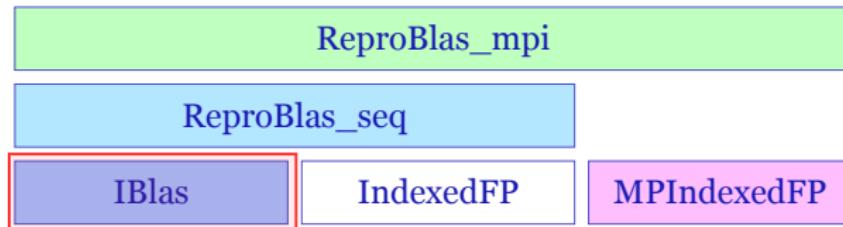


MPIIndexedFP is an MPI wrapper for IndexedFP:

- ▶ Data types: MPI_IDOUBLE, MPI_IFLOAT,
MPI_IDOUBLE_COMPLEX, MPI_ICOMPLEX
- ▶ Reduction operators: MPI_RSUM, MPI_RNRM2

ReproBLAS: Reproducible Basic Linear Algebra Subprograms

URL: <http://bebop.cs.berkeley.edu/reproblas>

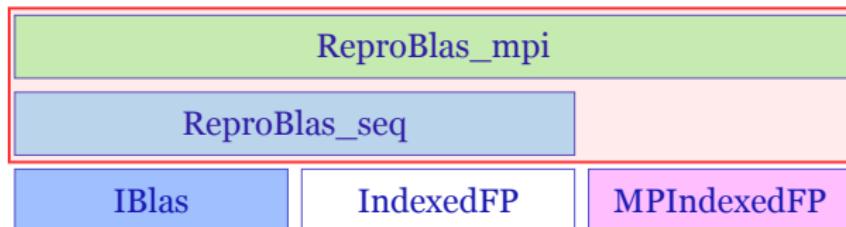


IBlas (Indexed Blas) provides performance-optimized kernel routines which take in vectors in native data type and return result in Indexed Floating Point format

- ▶ $\{s|d|c|z\} \text{asumI}$
- ▶ $\{s|d|c|z\} \text{sumI}$
- ▶ $\{s|d|c|z\} \text{nrm2I}$
- ▶ $\{s|d|c|z\} \text{dot}\{\text{c|u}\}\text{I}$

ReproBLAS: Reproducible Basic Linear Algebra Subprograms

URL: <http://bebop.cs.berkeley.edu/reproblas>



Current version only supports level 1 routines for 4 basic data types:

- ▶ $\{r|pr\}\{s|d|c|z\}$ `asum`
- ▶ $\{r|pr\}\{s|d|c|z\}$ `sum`
- ▶ $\{r|pr\}\{s|d|c|z\}$ `nrm2`
- ▶ $\{r|pr\}\{s|d|c|z\}$ `dot` $\{c|u\}$

Example 1: sum of sines

```
// Compute sum of sin(2*M_PI*(i/(double)n-0.5))

double sumsin(int n) {
    int i;
    double t;
    double s;

    s = 0.0;

    for ( i = 0; i < n; i++) {
        t = sin(2*M_PI*(i/(double)n-0.5));
        s = s + t;
    }

    return s;
}
```

Example 1: sum of sines (Reproducible)

```
#include <IndexedFP.h>

double sumsin(int n) {
    int i;
    double t;
    Idouble s;      // declare an indexed fp

    s = 0.0;

    for (i = 0; i < n; i++) {
        t = sin(2*M_PI*(i/(double)n-0.5));
        s = s + t;
    }

    return s;
}
```

Example 1: sum of sines (Reproducible)

```
#include <IndexedFP.h>

double sumsin(int n) {
    int i;
    double t;
    Idouble s;      // declare an indexed fp

    dISetZero(s); // Initialize to zero

    for ( i = 0; i < n; i++) {
        t = sin(2*M_PI*(i/(double)n-0.5));
        s = s + t;
    }

    return s;
}
```

Example 1: sum of sines (Reproducible)

```
#include <IndexedFP.h>

double sumsin(int n) {
    int i;
    double t;
    Idouble s;      // declare an indexed fp

    dISetZero(s); // Initialize to zero

    for ( i = 0; i < n; i++) {
        t = sin(2*M_PI*(i/(double)n-0.5));
        dIAddd(&s,t);      // Aggregation
    }

    return s;
}
```

Example 1: sum of sines (Reproducible)

```
#include <IndexedFP.h>

double sumsin(int n) {
    int i;
    double t;
    Idouble s;      // declare an indexed fp

    dISetZero(s); // Initialize to zero

    for ( i = 0; i < n; i++) {
        t = sin(2*M_PI*(i/(double)n-0.5));
        dIAddd(&s,t);      // Aggregation
    }

    return Iconv2d(s); // convert back to normal FP
}
```

Example 1: sum of sines (Parallel Reproducible)

```
#include <MPIIndexedFP.h>

double sumsin(int n) {
    int i;
    double t;
    Idouble s, s1;      // declare an indexed fp

    /* PARTITIONING. Local work: from start to end */

    dISetZero(s); // Initialize to zero
    for (i = start; i < end; i++) {
        t = sin(2 * M_PI * (i / (double) n - 0.5));
        dIAddd(&s, t); // Aggregation
    }

    RMPI_Init(); // Initialize Reproducible MPI
    MPI_Reduce(&s, &s1, 1, MPI_IDOUBLE, MPI_RSUM,
               0, MPI_COMM_WORLD);

    return Iconv2d(s1); // convert back to normal FP
}
```

Example 2: vector summation (naive)

```
int n = 1000000;
double* v = (double*)malloc(n*sizeof(double));

for (i=0;i<n;i++) v[i]=sin(2*M_PI*(i/(double)n-0.5));

double sum(int n, double* v) {
    int i;
    double t;
    double s;

    s = 0;           // Initialize to zero

    for ( i = 0; i < n; i++)
        s += v[i];

    return s;
}
```

Example 2: vector summation (reproducible)

```
#include <IndexedFP.h>

int n = 1000000;
double* v = (double*) malloc(n*sizeof(double));

for (i=0;i<n;i++) v[i]=sin(2*M_PI*(i/(double)n-0.5));

double sum_I(int n, double* v) {
    int i;
    double t;
    Idouble s;      // declare an indexed fp

    dISetZero(s); // Initialize to zero

    for ( i = 0; i < n; i++)
        dIAddd(&s,v[i]); // Aggregation

    return Iconv2d(s); // convert back to normal FP
}
```

Example 2: vector summation (reproducible blas)

```
#include <rblas.h>

int n = 1000000;
double* v = (double*) malloc(n*sizeof(double));

for (i=0;i<n;i++) v[i]=sin(2*M_PI*(i/(double)n-0.5));

extern double rdsum(int n, double* v, int inc);

double sum_I(int n, double* v) {
    return rdsum(n, v, 1);
}
```

Example 2: vector summation (parallel reproducible blas)

```
#include <rblas_mpi.h>

// double* v : local vector
// int n      : length of local vector

extern double prdsum(MPI_Comm* com, int root,
                      int n, double* v, int inc);

double sum_I(int n, double* v) {
    return prdsum(MPI_COMM_WORLD, 0, n, v, 1);
}
```

Example 2: vector summation (blocked)

```
#include <IndexedFP.h>
#define NB 1024
int n = 1000000;
// v[i] = sin(2*M_PI*(i/(double)n-0.5)

double sum_I(int n, double* v) {
    int i, LN;
    double t;
    Idouble s;      // declare an indexed fp
    dISetZero(s); // Initialize to zero
    for ( i = 0; i < n; i += NB, v += NB) {
        LN = NB < (n-i) ? NB : (n-i);
        dIAddd(&s,sum(LN,v)); // Block Aggregation
    }
    return Iconv2d(s); // convert back to normal FP
}
```

Example 1: sum of sines (Revisited)

```
#include <rblas.h>

#define NB 128
double sumsin(int n) {
    int i, j;
    double t;
    Idouble s, s1;      // declare an indexed fp
    double BUFFER[NB];

    dISetZero(s); // Initialize to zero

    for (i = 0; i < n; i+=NB) {
        lN = NB < (n-i) ? NB : (n-i);
        for (j = 0; j < lN; j++)
            BUFFER[j] = sin(2*M_PI*((i + j)/(double)n-0.5));
        s1 = dsumI(lN, BUFFER, 1); // Indexed BLAS call
        dIAAdd(&s, s1);         // Aggregation
    }

    return Iconv2d(s); // convert back to normal FP
}
```

Development status

<http://bebop.cs.berkeley.edu/reproblas>

x: complete o: in progress

		Single-threaded			Multi-threaded		GPU	MPI	...
		Scalar	SSE	AVX	OMP	pthread			
BLAS 1	asum	x	x	o	o			x	
	sum	x	x	o	o			x	
	dot	x	x	o	o			x	
	nrm2	x	x	o	o			x	
2	gemv	o	o						
	trsv	o	o						
3	gemm								
	trsm								

Future work: LAPACK, hardware support, non-linear operations, ...