Efficient, Optimal MPI Datatype Reconstruction for Vector and Index Types

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MPI Derived datatypes

...you all know about them

Mechanism for describing application data layouts that are

• Non-consecutive (sub-matrices, parts of buffers, ...)
• Non-homogeneous: different basetypes (MPI_CHAR, MPI_DOUBLE, MPI_INT, ...)

Derived (user-defined) datatypes orthogonal to communication mode: works for point-to-point, collective, one-sided, extremely important for MPI-IO specification, ...

Unique feature of MPI (could be useful for other interfaces!)
**Example:** Receive two matrix-column blocks...

Rowtype = MPI_Indexed

BlocksType = MPI_Contig(Rowtype)

Note: BlocksType ≠ BlocksType'

BlocksType' = MPI_Struct(Column1,Column2)
**Note:** BlocksType ≠ BlocksType’

Derived datatype describes the *layout* of data, and fixes the *order* in which data are accessed.

**Layout:** *Ordered sequence* of `<displacement, basetype> pairs`  

*aka MPI type map*

**Example:** The row-wise layout of matrix-columns:

```plaintext
<10,DOUBLE>, <11,DOUBLE>, <20,DOUBLE>, <21,DOUBLE>,  
<22,DOUBLE>, <110,DOUBLE>, <111,DOUBLE>, <120,DOUBLE>,  
<121,DOUBLE>, <122,DOUBLE>, ...
```
Note: BlocksType ≠ BlocksType’

Derived datatype describes the **layout** of data, and fixes the **order** in which data are accessed.

**Layout**: Ordered sequence of `<displacement, basetype>` pairs

*Homogeneous*: same basetype for all pairs  
aka MPI type map

**Example**: Row-wise layout of matrix-columns, basetype DOUBLE

`<10,11,20,21,22,110,111,120,121,122, ...>`

**Displacement sequence**: list of displacements (in access order)

Displacements themselves not necessarily ordered!
Note: BlocksType ≠ BlocksType’

Derived datatype describes the layout of data, and fixes the order in which data are accessed

Layout: Ordered sequence of <displacement, basetype> pairs

Homogeneous: same basetype for all pairs

aka MPI type map

Example: Column-wise layout of matrix-columns

<10,11,110,111,210,211,…,20,21,22,120,121,122,220,221,222, …>

Displacement sequence: list of displacements (in access order)

Displacements themselves not necessarily ordered!
Datatype representation

Tree (or DAG) like structure:

• Internal type nodes describe how child nodes are repeated (how often, where)
• Leaf nodes describe basetype

Semantics:
There is a function flatten(T) that generates the type map from datatype T, i.e., flatten(T) = D

MPI usage:
Derived datatype explicitly constructed by application using type constructor operations, MPI library maintains some convenient and efficient internal representation
Derived datatype representation of displacement sequence

\[
\begin{align*}
\text{MPI\_Contig}(60) & \quad \downarrow \\
\text{MPI\_Indexed}(2,\langle 2,3 \rangle) & \quad \downarrow \\
\text{MPI\_DOUBLE} & \\
\end{align*}
\]

Type nodes:
- MPI\_Contig
- MPI\_Vector
- MPI\_IndexBlock
- MPI\_Indexed

MPI datatype constructors
- MPI\_Type\_contiguous(oldtype, ..., &newtype);
- MPI\_Type\_vector(oldtype, ..., &newtype);
- MPI\_Type\_create\_indexed\_block(oldtype, ..., &newtype);
- MPI\_Type\_indexed(oldtype, ..., &newtype);
Derived datatype representation of heterogeneous type map

Type nodes:
- MPI_Type_contiguous
- MPI_Type_vector
- MPI_Type_create_indexed_block
- MPI_Type_indexed
- MPI_Type_create_struct

MPI datatype constructors

- MPI_Type_contiguous(oldtype, ..., &newtype);
- MPI_Type_vector(oldtype, ..., &newtype);
- MPI_Type_create_indexed_block(oldtype, ..., &newtype);
- MPI_Type_indexed(oldtype, ..., &newtype);
- MPI_Type_create_struct(oldtypes[], ..., &newtype);
Derived datatype representation of heterogeneous type map

Type nodes:
- MPI_Contig
- MPI_Vector
- MPI_IndexBlock
- MPI_Indexed
- MPI_Struct

MPI datatype constructors

- `MPI_Type_contiguous(oldtype, ..., &newtype);`
- `MPI_Type_vector(oldtype, ..., &newtype);`
- `MPI_Type_create_indexed_block(oldtype, ..., &newtype);`
- `MPI_Type_indexed(oldtype, ..., &newtype);`
- `MPI_Type_create_struct(oldtypes[], ..., &newtype);`
Our internal representation (not very important here)

• leaf(B): basetype B at displacement 0
• vec(c,d,C): regular, strided repetition of subtype C at displacements 0, d, 2d, 3d, ... (c-1)d
• idx(c,<i0,i1,i2,...,i(c-1)>,C): repetition of subtype C at displacements i0, i1, i2, ..., i(c-1)

• strc(c,<i0,i1,i2,...,i(c-1)>,<C0,C1,C2,...,C(c-1)>): subtypes C0, C1, C2, ..., C(c-1) at displacements i0, i1, i2, ..., i(c-1)

• Can easily represent the MPI constructors (for now, we omit MPI_Type_indexed)
• Avoids some tedious problems with extents and “true extents”
Datatype representation

Tree (or DAG) like structure:

- Internal type nodes describe how child nodes are repeated (how often, where)
- Leaf nodes describe basetype

**Semantics:**
There is a function flatten(T) that generates the type map from datatype T, i.e., flatten(T) = D

**Note:**
There are (infinitely) many ways T to describe a given D

Some may be better than others
Some natural questions

• What is the best way to describe given displacement sequence (homogeneous type map) as derived datatype?

• What is the best way to describe heterogeneous type map as derived datatype?

• How do the set of constructors affect complexity and quality?

Depends on what is meant by “best” (cost function)

Abstract cost function:
Account for space consumption and (indirectly) processing cost

Real “best” depends on MPI library and (communication) system
Cost model

- \(\text{cost(leaf}(B))\): some constant \(K\)
- \(\text{cost(vec}(c,d,C))\): some (other) constant \(K'\)
- \(\text{cost(idx}(c,<i_0,i_1,i_2,\ldots,i_{(c-1)},C))\): some constant \(K''+c\) (non-constant)

- \(\text{cost(strc}(c,<i_0,i_1,i_2,\ldots,i_{(c-1)},<C_0,C_1,C_2,\ldots,C_{(c-1)}))\): some constant \(K'''+2c\) (non-constant)

**Justification:**
leaf, vec: only constant information needed to process
idx, struc: space proportional to displacement and type lists required, must be traversed on processing

\(\text{cost}(T)\): sum of costs of all nodes in \(T\) (additive cost model)
Problems

Given:
• set of constructors (leaf, vec, idx, struc, …)
• cost function cost(T)

Type reconstruction problem: Find cost-optimal representation for given type map
Type normalization problem: Find cost-optimal representation for given, user-defined datatype

**Known facts**

MPI libraries use heuristics (*folklore*) to improve internal datatype representation: type normalization, *see, e.g.*, Fredrik Kjolstad, Torsten Hoefler, Marc Snir: Automatic datatype generation and optimization. PPOPP 2012: 327-328 (*and more extensive TR!*)

Homogeneous type maps of size $n$, *leaf*, *vec* and *idx* nodes: $O(n\sqrt{n})$ time reconstruction, normalization in time $O(\text{size}(T))$

Jesper Larsson Träff: Optimal MPI Datatype Normalization for Vector and Index-block Types. EuroMPI/ASIA 2014: 33
New results

Homogeneous type maps of size n, leaf, vec and idx nodes:
Better algorithm for finding all repeated prefixes, $O(n \log n/\log \log n)$ time type reconstruction
• Prefix algorithm can be used for normalization
• MPI_Index (idxbuc node) can be incorporated in $O(n^2 \log^2 n)$ time

Not here:
Arbitrary type maps of size n, all type nodes leaf, vec, idx, struc, type reconstruction into trees is polynomial but $O(n^4)$


and Master’s Thesis by Martin Kalany
Type reconstruction strategy

Derived datatype nodes describe structured repetition of subtype

To compute datatype from given displacement sequence: look for all possible repetitions

Use dynamic programming to compute best datatype

From now on: homogeneous type maps = displacement sequences
Terminology

**Displacement sequence:**
Array $D[]$ of $n$ integer displacements, $D[i]$ $i$'th displacement in sequence ($D[i]$ can be $>0$, $<0$, $=0$, repetitions allowed)

$$D[] = <10,11,20,21,22,110,111,120,121,122, ...>$$

...can trivially be represented as derived datatype

$$\text{idx}(n, <10,11,20,21,22,110,111,120,121,122, ...>)$$

\[ \downarrow \]

**DOUBLE**

Cost = $n + K'' + K$
Terminology

Displacement sequence:
Array D[] of n integer displacements, D[i] i’th displacement in sequence (D[i] can be >0, <0, =0, repetitions allowed)

D[] = <10,11,20,21,22,110,111,120,121,122, ...>

D[i,j]: Segment of displacement sequence from i to j (inclusive)

D[2,4] = <20,21,22>       D[0,2] = <10,11,20>

D[0,p-1]: Prefix of length p
**Definition:**
Prefix of length \( p \) is **repeated** in \( D \) if

\[
D[j] - D[0] = D[ip+j] - D[ip]
\]

for \( 0 \leq j < p \) and \( 1 \leq i < n/p \)

**Observation:** A prefix of length \( p \) can be repeated only if \( p \mid n \),
trivial prefixes \( D[0,0] \) of length 1 and \( D[0,n-1] \) of length 1

**Definition:** A repeated prefix of length \( p \) is **strided** if additionally

\[
D[p] - D[0] = D[(i+1)p] - D[ip]
\]
Prefix $D[0,4] = \{10,11,20,21,22\}$ is repeated (and strided) in $D[] = \{10,11,20,21,22,110,111,120,121,122, \ldots\}$

\[
\begin{array}{cccc}
0^+ & 100^+ & 200^+ & \text{strided} \\
10,11,20,21,22 & 10,11,20,21,22 & 10,11,20,21,22 & \ldots
\end{array}
\]

\[
\text{vec}(n/5,100) \\
\text{idx}(5,\{10,11,20,21,22\}) \\
\text{DOUBLE}
\]

Cost $= K' + 5 + K'' + K$
Finding repeated prefixes

Finding *strided* prefixes is easy (EuroMPI 2014): longest repeated prefix in arbitrary D can be found in one scan in \(O(n)\) time.

Finding repeated, non-strided prefixes; trivial approach:

Try all divisors \(p\) of \(n\), for each check by scan of \(D\) whether prefix \(D[0,p-1]\) is repeated: total time \(O(n\sqrt{n})\)

**Observation:**
If \(D[0,p-1]\) is repeated prefix of \(D\), checking whether \(D[0,p-1]\) is a strided prefix takes \(O(n/p)\) time.
**Claim:**
Let p divisor of n. All repeated prefixes of length q where q is a divisor of p (including q=p) can be found in linear time.

**Idea:**
To find all repeated prefixes of D, let

\[ n = (p_1^{a_1}) (p_2^{a_2}) (p_3^{a_3}) \ldots (p_k^{a_k}) \]

be prime factorization of n. Apply claim for all \( p = (n/pi) \)

Result from number theory (Robin, 1983):

Number of distinct prime factors of n is \( O(\log n/\log \log n) \)
Proposition:
All repeated prefixes of given displacement sequence D of length n can be found in $O(n \log n / \log \log n)$ time.

Proof of claim:
Pick (largest) divisor $p$ of $n$, check if $D[0,p-1]$ is repeated prefix.

Prefix mismatch:
$D[ip+j] - D[ip] \neq D[j] - D[0]$
Prefix mismatch: 
\[ D[ip+j] - D[ip] \neq D[j] - D[0] \]

1. Choose \( p' = \gcd(p, j) \), continue scan for repeated prefix 
\[ D[0, p'-1] \] from \( j \)

Prefix that is divisor of \( p \) but not \( j \) cannot be repeated prefix
Prefix mismatch: $D[ip+j]-D[ip] \neq D[j]-D[0]

1. Choose $p' = \gcd(p, j)$, continue scan for repeated prefix $D[0,p'-1]$ from $j$
2. Check whether prefix $D[0,p'-1]$ is repeated in $D[0,p-1]$

Step 2: recurse on $p'$ in $p$
Prefix mismatch: \[ D[ip+j] - D[ip] \neq D[j] - D[0] \]

Step 1: linear scan, always increasing index order: \( O(n) \)

Step 2: recurse on \( p' \) in \( p \) so \( O(p) \)

Total time: \( O(n) \)
Prefix mismatch: $D[ip+j]-D[ip] \neq D[j]-D[0]$

Algorithm determines largest $p'$ that is a divisor of $p$ where $D[0,p'-1]$ is repeated prefix of $D$
Prefix mismatch:
\( D[ip+j] - D[ip] \neq D[j] - D[0] \)

To find all repeated prefixes of length \( q \) where \( q \) divisor of \( p \):
recurse on \( q \) in \( p \).

Observation:
If \( D[0,q-1] \) is repeated prefix of \( D[0,p-1] \), and \( D[0,p-1] \) is repeated prefix of \( D \), then \( D[0,q-1] \) is repeated prefix of \( D \)
Structure of optimal path

Observations:
With leaf, vec, idx nodes (no struc), datatypes are simple paths. Each constructor has only one child

Call index node \( \text{idx}(c,\langle i_0, i_1, \ldots \rangle) \) where \( i_0 \neq 0 \) a shifted node. A type tree with at most one shifted node is nice. For any datatype path \( T \) there exists nice \( T' \) (describing the same displacement sequence) with \( \text{cost}(T') \leq \text{cost}(T) \)

Cost-optimal \( T \) has at most one node with count=1 (a shifted idx)

Cost optimal \( T \) has depth (log \( n \))

Cost optimal \( T \)'s have optimal substructure: dynamic programming principle applies
\[
\text{idx}(1, \langle 0 \rangle) \\
\downarrow \\
\text{idx}(3, \langle 27, 2, 55 \rangle) \\
\downarrow \\
\text{idx}(2, \langle 0, 7, 13 \rangle) \\
\downarrow \\
\text{idx}(3, \langle 1, 2, 4 \rangle) \\
\downarrow \\
\text{DOUBLE}
\]

\[
\text{idx}(1, \langle 28 \rangle) \\
\downarrow \\
\text{idx}(3, \langle 0, -25, 28 \rangle) \\
\downarrow \\
\text{idx}(2, \langle 0, 7, 13 \rangle) \\
\downarrow \\
\text{idx}(3, \langle 0, 1, 3 \rangle) \\
\downarrow \\
\text{DOUBLE}
\]
Full algorithm

Precompute: all repeated prefixes and longest strides

1. Find all repeated prefixes $p$
2. For each $p$, find largest $s(p) \leq n$ such that $D[0,p-1]$ is strided in $D[0,s(p)-1]$
3. Optimal datatype representation for segment $D[0,0]$ of length 1 is $T(0) = \text{leaf(basetype)}$

Technicality:
Algorithm for aligned displacement sequences with $D[0] = 0$
Step 4: dynamic programming

for all repeated prefixes D[0,p-1]:
    BestCost = ∞
for all repeated prefixes q of D[0,p-1]:

    VecCost = K' + cost(T(q)) // cost of vec node
    if VecCost < BestCost and p ≤ s(q)
        T(p) = vec(p/q, stride, T(q)) where stride = D[q] - D[0]
        BestCost = VecCost

    IdxCost = K'' + p/q + cost(T(q)) // cost of idx node
    if IdxCost < BestCost
        indices = <D[0], D[q], D[2q],...>
        T(p) = idx(p/q, indices, T(q))
        BestCost = IdxCost
Complexity

Steps 1 takes $O(n \log n / \log \log n)$ time by the proposition on repeated prefixes.

Step 2 requires $O(n/p)$ time for each divisor $p|n$. By a theorem from number theory (Divisor summatory function, Gronwall, 1913)

$$\sum(p|n): n/p = \sum(p|n): p = O(n \log n / \log \log n)$$

In step 4, both loops are over repeated prefixes. There can be at most $2\sqrt{n}$, so if body of inner loop can be implemented in constant time, total time is $O(n)$.
for all repeated prefixes \(D[0,p-1]\):

\[
\text{BestCost} = \infty
\]

for all repeated prefixes \(q\) of \(D[0,p-1]\):

\[
\text{VecCost} = K' + \text{cost}(T(q)) \quad // \text{cost of vec node}
\]

if \(\text{VecCost} < \text{BestCost}\) and \(p \leq s(q)\)

\[
T(p) = \text{vec}(p/q, \text{stride}, T(q)) \quad \text{where stride} = D[q] - D[0]
\]

\[
\text{BestCost} = \text{VecCost}
\]

\[
\text{IdxCost} = K'' + \frac{p}{q} + \text{cost}(T(q)) \quad // \text{cost of idx node}
\]

if \(\text{IdxCost} < \text{BestCost}\)

\[
\text{indices} = <D[0],D[q],D[2q],...>
\]

\[
T(p) = \text{idx}(p/q, \text{indices}, T(q))
\]

\[
\text{BestCost} = \text{IdxCost}
\]

Fill in indices later
Theorem:
Cost optimal datatype path representing displacement sequence $D$ of length $n$ using constructors leaf, vec, idx can be computed in $O(n \log n / \log \log n)$ time
Additional constructors

idx node corresponds to MPI_Type_create_indexed_block constructor.

MPI_Type_indexed needs list of displacements and list of block sizes, represented by additional constructor

\[ \text{idxbuc}(c,d,<i_0,i_1,i_2,\ldots,i_{c-1}>,<b_0,b_1,b_2,\ldots,b_{c-1}>) \text{ with cost } K'' + 2c \]

Extra check in inner loop of dynamic programming algorithm needed, requires sorting (to find best block size), total time \( O(\sqrt{n}n \log n) \)
Outlook, summary

• Simple algorithm to find all repeated prefixes much faster than trivial $O(n\sqrt{n})$ approach

• Much better algorithm for type reconstruction with restricted set of constructors leaf, vec, idx, now $O(n \log n / \log \log n)$

• Can be used in algorithm for type normalization (EuroMPI 2014)

• Can incorporate additional constructors: idxbuc (MPI_Type_indexed), triangular types (see tomorrow), ..., but not for type normalization
Note: `struc()` node does give more power, even for (homogeneous) displacement sequences

\[
\text{idx}(1,\langle 0,1,2,3,4,5,100,102,104,\ldots,120 \rangle) \rightarrow \text{INT}
\]

\[
\text{struc}(2,\langle 0,100 \rangle) \rightarrow \text{INT}
\]

\[
\text{vec}(6,1) \rightarrow \text{vec}(11,2) \rightarrow \text{INT}
\]

Cost = \( K'' + 17 + K \)

Cost = \( K''' + 2 + 2K' + K \)

Makes sense to look for constructors in between `idx()` and `struc()`.
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EPiGRAM