

TcIMPI

1.1

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Chapter 1

Main Page

The TcIMPI package contains software that wraps an MPI library for Tcl and allows MPI calls to be used from Tcl scripts. This code can be compiled as a shared object to be loaded into an existing Tcl interpreter or as a standalone TcIMPI interpreter. In combination with some additional bundled Tcl script code, additional commands are provided that allow to run Tcl scripts in parallel via "mpirun" or "mpiexec" similar to C, C++ or Fortran programs.

1.0.1 Homepage:

The main author of this package is Axel Kohlmeyer and you can reach him at akohlmey@gmail.com. The official homepage for this project is <https://akohlmey.github.io/tclmpi/> and development is hosted on GitHub.

For basic compilation and installation instructions, please see the file INSTALL. More detailed documentation is available online from the [User's Guide](#).

Information about the implementation and design of the package are in the [Developer's Guide](#).

1.0.2 Test Status:

1.0.3 Citing:

You can cite TcIMPI as:

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1.0.4 Acknowledgements:

Thanks to Arjen Markus and Chris MacDermaid for encouragement and (lots of) constructive criticism, that has helped enormously to develop the package from a crazy idea to its current level. Thanks to Alex Baker for motivating me to convert to using CMake as build system which makes building TcIMPI natively on Windows much easier.

A special thanks also goes to Karolina Sarnowska-Upton and Andrew Grimshaw that allowed me to use TcIMPI as an example in their MPI portability study, which helped to find quite a few bugs and resolve several portability issues before the code was hitting the real world.

Chapter 2

Copyright and License for TcIMPI

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Chapter 3

TclMPI User's Guide

This page describes Tcl bindings for MPI. This package provides a shared object that can be loaded into a Tcl interpreter to provide additional commands that act as an interface to an underlying MPI implementation. This allows to run Tcl scripts in parallel via `mpirun` or `mpiexec` similar to C, C++ or Fortran programs and communicate via wrappers to MPI function call.

The original motivation for writing this package was to complement a Tcl wrapper for the LAMMPS molecular dynamics simulation software, but also allow using the VMD molecular visualization and analysis package in parallel without having to recompile VMD and using a convenient API to people that already know how to program parallel programs with MPI in C, C++ or Fortran.

3.1 Compilation and Installation

The package currently consist of a single C source file which usually will be compiled for dynamic linkage, but can also be compiled into a new Tcl interpreter with TclMPI included (required on some platforms that require static linkage) and a Tcl script file. In addition the package contains some examples, a simple unit test harness (implemented in Tcl) and a set of tests to be run with either one MPI rank (`test01`, `test02`) or two MPI ranks (`test03`, `test04`).

The build system uses CMake (version 3.16 or later) and has been confirmed to work on Linux macOS and Windows. The MPI library has to be at least MPI-2 standard compliant and the Tcl version should be 8.6 or later (it may work with 8.5, too). When compiled for a dynamically loaded shared object (DSO) or DLL file, the MPI library has to be compiled and linked with support for building shared libraries as well (this is the default for OpenMPI on Linux, but your mileage may vary).

To configure and build TclMPI you need to run CMake the usual way, for example with

```
cmake -B build-folder -S .
cmake --build build-folder
cmake --install build-folder
```

There are a few settings that can be used to adjust what is compiled and installed and where. The following settings are supported:

- `BUILD_TCLMPI_SHELL` Build a `tclmpish` executable as extended Tcl shell (default: on)
- `ENABLE_TCL_STUBS` Use the Tcl stubs mechanism (default: on, requires Tcl 8.6 or later)
- `BUILD_TESTING` Enable unit testing (default: on)
- `DOWNLOAD_MPICH4WIN` Download MPICH2-1.4.1 headers and link library (default: off, Windows only)

- CMAKE_INSTALL_PREFIX Path to installation location prefix (default: (platform specific))

To change settings from the defaults append `-D<SETTING>=<VALUE>` to the `cmake` command line and replace `<SETTING>` and `<VALUE>` accordingly.

To enable the new TclMPI package you can use the command `set auto_path [concat /usr/local/tcl8.6/$auto_path]` in your `.tclshrc` (or `.vmdrc` or similar) file and then you can load the TclMPI wrappers on demand simply by using the command `package require tclmpi`. For the extended shell, the `_tclmpi.so` file is not used and instead `tclmpish` needs to run instead of `tclsh`. For that you may append the `bin` folder of the installation tree to your `PATH` environment variable. In case of using the custom Tcl shell, the startup script would be called `.tclmpishrc` instead of `.tclshrc`.

3.2 Software Development and Bug Reports

The TclMPI code is maintained using git for source code management, and the project is hosted on github at <https://github.com/akohlmeier/tclmpi>. From there you can download snapshots of the development and releases, clone the repository to follow development, or work on your own branch through forking it. Bug reports and feature requests should also be filed on github at through the issue tracker at: <https://github.com/akohlmeier/tclmpi/issues>.

3.3 Example Programs

The following section provides some simple examples using TclMPI to recreate some common MPI example programs in Tcl.

3.3.1 Hello World

This is the TclMPI version of "hello world".

```
#!/bin/sh \
exec tclsh "$0" "$@"
package require tclmpi 1.1
# initialize MPI
::tclmpi::init
# get size of communicator and rank of process
set comm tclmpi::comm_world
set size [::tclmpi::comm_size $comm]
set rank [::tclmpi::comm_rank $comm]
puts "hello world, this is rank $rank of $size"
# shut down MPI
::tclmpi::finalize
exit 0
```

3.3.2 Computation of Pi

This script uses TclMPI to compute the value of Pi from numerical quadrature of the integral:

$$\pi = \int_0^1 \frac{4}{1+x^2} dx$$

```
#!/bin/sh \
exec tclsh "$0" "$@"
package require tclmpi 1.1
# initialize MPI
::tclmpi::init
set comm tclmpi::comm_world
set size [::tclmpi::comm_size $comm]
```

```

set rank [::tclmpi::comm_rank $comm]
set master 0
set num [lindex $argv 0]
# make sure all processes have the same interval parameter
set num [::tclmpi::bcast $num ::tclmpi::int $master $comm]
# run parallel calculation
set h [expr {1.0/$num}]
set sum 0.0
for {set i $rank} {$i < $num} {incr i $size} {
    set sum [expr {$sum + 4.0/(1.0 + ($h*($i+0.5))*2)}]
}
set mypi [expr {$h * $sum}]
# combine and print results
set mypi [::tclmpi::allreduce $mypi tclmpi::double \
    tclmpi::sum $comm]
if {$rank == $master} {
    set rel [expr {abs(($mypi - 3.14159265358979)/3.14159265358979)}]
    puts "result: $mypi. relative error: $rel"
}
# shut down MPI
::tclmpi::finalize
exit 0

```

3.3.3 Distributed Sum

This is a small example version that distributes a data set and computes the sum across all elements in parallel.

```

#!/bin/sh \
exec tclsh "$0" "$@"
package require tclmpi 1.1
# data summation helper function
proc sum {data} {
    set sum 0
    foreach d $data {
        set sum [expr {$sum + $d}]
    }
    return $sum
}
::tclmpi::init
set comm $tclmpi::comm_world
set mpi_sum $tclmpi::sum
set mpi_double $tclmpi::double
set mpi_int $tclmpi::int
set size [::tclmpi::comm_size $comm]
set rank [::tclmpi::comm_rank $comm]
set master 0
# The master creates the list of data
#
set dataSize 1000000
set data {}
if { $comm == $master } {
    set mysum 0
    for { set i 0 } { $i < $dataSize } { incr i } {
        lappend data $i
    }
}
# add padding, so the number of data elements is divisible
# by the number of processors as required by tclmpi::scatter
set needpad [expr {$dataSize % $size}]
set numpad [expr {$needpad ? ($size - $needpad) : 0}]
if { [comm_rank $comm] == $master } {
    for {set i 0} {$i < $numpad} {incr i} {
        lappend data 0
    }
}
set blocksz [expr {($dataSize + $numpad) / $size}]
# distribute data and do the summation on each node
# the sum the result across all nodes. Note: the data
# is integer, but we need to do the full sum in double
# precision to avoid overflows.
set mydata [::tclmpi::scatter $data $mpi_int $master $comm]
set sum [::tclmpi::allreduce [sum $mydata] $mpi_double $mpi_sum $comm]
if { $comm == $master } {
    puts "Distributed sum: $sum"
}
::tclmpi::finalize

```


Chapter 4

TclMPI Developer's Guide

This document explains the implementation of the Tcl bindings for MPI implemented in TclMPI. The following sections will document how and which MPI is mapped to Tcl and what design choices were made.

4.1 Overall Design and Differences to the MPI C-bindings

To be consistent with typical Tcl conventions all commands and constants in lower case and prefixed with `tclmpi`, so that clashes with existing programs are reduced. This is not yet set up to be a proper namespace, but that may happen at a later point, if the need arises. The overall philosophy of the bindings is to make the API similar to the MPI one (e.g. maintain the order of arguments), but don't stick to it slavishly and do things the Tcl way wherever justified. Convenience and simplicity take precedence over performance. If performance matters that much, one would write the entire code C/C++ or Fortran and not Tcl. The biggest visible change is that for sending data around, receive buffers will be automatically set up to handle the entire message. Thus the typical "count" arguments of the C/C++ or Fortran bindings for MPI is not required, and the received data will be the return value of the corresponding command. This is consistent with the automatic memory management in Tcl, but this convenience and consistency will affect performance and the semantics. For example calls to `tclmpi::bcast` will be converted into *two* calls to `MPI_Bcast()`; the first will broadcast the size of the data set being sent (so that a sufficiently sized buffers can be allocated) and then the second call will finally send the data for real. Similarly, `tclmpi::recv` will be converted into calling `MPI_Probe()` and then `MPI_Recv()` for the purpose of determining the amount of temporary storage required. The second call will also use the `MPI_SOURCE` and `MPI_TAG` flags from the `MPI_Status` object created for `MPI_Probe()` to make certain, the correct data is received.

Things get even more complicated with with non-blocking receives. Since we need to know the size of the message to receive, a non-blocking receive can only be posted, if the corresponding send is already pending. This is being determined by calling `MPI_Iprobe()` and when this shows no (matching) pending message, the parameters for the receive will be cached and the then `MPI_Probe()` followed by `MPI_Recv()` will be called as part of `tclmpi::wait`. The blocking/non-blocking behavior of the Tcl script should be very close to the corresponding C bindings, but probably not as efficient.

4.2 Naming Conventions

All functions that are new Tcl commands follow the MPI naming conventions, but using `TclMPI_` as prefix instead of `MPI_`. The corresponding Tcl commands are placed in the `tclmpi` namespace and all lower case. Example: `TclMPI_Init()` is the wrapper for `MPI_Init()` and is provided as command `tclmpi::init`. Defines and constants from the MPI header file are represented in TclMPI as plain strings, all lowercase and with a `tclmpi::` prefix. Thus `MPI_COMM_WORLD` becomes `tclmpi::comm_world` and `MPI_INT` becomes `tclmpi::int`.

Functions that are internal to the plugin as well as static variables are prefixed with all lower case, i.e. `tcimpi_`. Those functions have to be declared static.

All string constants are also declared as namespace variables, e.g. `$tcimpi::comm_world`, so that shortcut notations are possible as shown in the following example:

```
namespace upvar tcimpi comm_world comm
namespace upvar tcimpi int mpi_int
```

4.3 TclMPI Support Functions

Several MPI entities like communicators, requests, status objects cannot be represented directly in Tcl. For TclMPI they need to be mapped to something else, for example a string that will uniquely identify this entity and then it will be translated into the real object it represents with the help of the following support functions.

4.3.1 Mapping MPI Communicators

MPI communicators are represented in TclMPI by strings of the form `"tcimpi::comm%d"`, with `"%d"` being replaced by a unique integer. In addition, a few string constants are mapped to the default communicators that are defined in MPI. These are `tcimpi::comm_world`, `tcimpi::comm_self`, and `tcimpi::comm_null`, which represent `MPI_COMM_WORLD`, `MPI_COMM_SELF`, and `MPI_COMM_NULL`, respectively.

Internally the map is maintained in a simple linked list which is initialized with the three default communicators when the plugin is loaded and where new communicators are added at the end as needed. The functions `mpi2tcl_comm` and `tcl2mpi_comm` are then used to translate from one representation to the other while `tcimpi_add_comm` will append a new structure containing the communicator to the list. Correspondingly `tcimpi_del_comm` will remove a communicator entry from the list, based on its Tcl string representation.

4.3.2 Mapping MPI Requests

MPI requests are represented in TclMPI by strings of the form `"tcimpi::req%d"`, with `"%d"` being replaced by a unique integer. Internally this map is maintained in a simple linked list to which new requests are appended and from which completed requests are removed as needed. The function `tcimpi_find_req` is used to locate a specific request and its associated data from its string label. In addition, `tcimpi_add_req` will append a new request to the list, and `tcimpi_del_req` will remove (completed) requests.

4.3.3 Mapping Data Types

The helper function `tcimpi_datatype` is used to convert string constants representing specific data types into integer constants for convenient branching. Data types in TclMPI are somewhat different from MPI data types to match better the spirit of Tcl scripting.

4.3.4 Common Error Message Processing

There is a significant redundancy in checking for and reporting error conditions. For this purpose, several support functions exist.

`tcimpi_errcheck` verifies if calls to the MPI library were successful and if not, generates a formatted error message that is appended to the current result list.

`tcimpi_commcheck` verifies if a communicator argument was using a valid Tcl representation and if not, generates a formatted error message that is appended to the current result list.

`tcimpi_typecheck` test if a type argument was using a valid Tcl representation and if not, generates a formatted error message that is appended to the current result list.

Chapter 5

Namespace Index

5.1 Namespace List

Here is a list of all documented namespaces with brief descriptions:

tclmpi	15
tclmpi_test	29

Chapter 6

Class Index

6.1 Class List

Here are the classes, structs, unions and interfaces with brief descriptions:

tclmpi_comm	35
tclmpi_dblint	36
tclmpi_intint	37
tclmpi_req	38

Chapter 7

Namespace Documentation

7.1 tclmpi Namespace Reference

Functions

- proc [init](#) ()
- proc [initialized](#) ()
- proc [conv_set](#) (handler)
- proc [conv_get](#) (handler)
- proc [finalize](#) ()
- proc [finalized](#) ()
- proc [abort](#) (comm, errorcode)
- proc [comm_size](#) (comm)
- proc [comm_rank](#) (comm)
- proc [comm_split](#) (comm, color, key)
- proc [comm_free](#) (comm)
- proc [barrier](#) (comm)
- proc [bcast](#) (data, type, root, comm)
- proc [scatter](#) (data, type, root, comm)
- proc [allgather](#) (data, type, comm)
- proc [gather](#) (data, type, root, comm)
- proc [allreduce](#) (data, type, op, comm)
- proc [reduce](#) (data, type, op, root, comm)
- proc [send](#) (data, type, dest, tag, comm)
- proc [isend](#) (data, type, dest, tag, comm)
- proc [recv](#) (type, source, tag, comm, status={})
- proc [irecv](#) (type, source, tag, comm)
- proc [probe](#) (source, tag, comm, status={})
- proc [wait](#) (request, status={})
- proc [waitall](#) (requests, status={})

Variables

- variable `version` = "1.1"
version number of this package
- variable `auto` = `tcLmpi::auto`
constant for automatic data type
- variable `int` = `tcLmpi::int`
constant for integer data type
- variable `intint` = `tcLmpi::intint`
constant for integer pair data type
- variable `double` = `tcLmpi::double`
constant for double data type
- variable `dblint` = `tcLmpi::dblint`
constant for double/int pair data type
- variable `comm_world` = `tcLmpi::comm_world`
constant for world communicator
- variable `comm_self` = `tcLmpi::comm_self`
constant for self communicator
- variable `comm_null` = `tcLmpi::comm_null`
constant empty communicator
- variable `any_source` = `tcLmpi::any_source`
constant to accept messages from any source rank
- variable `any_tag` = `tcLmpi::any_tag`
constant to accept messages with any tag
- variable `sum` = `tcLmpi::sum`
summation operation
- variable `prod` = `tcLmpi::prod`
product operation
- variable `max` = `tcLmpi::max`
maximum operation
- variable `min` = `tcLmpi::min`
minimum operation
- variable `land` = `tcLmpi::land`
logical and operation
- variable `band` = `tcLmpi::band`
bitwise and operation
- variable `lor` = `tcLmpi::lor`
logical or operation
- variable `bor` = `tcLmpi::bor`
bitwise or operation
- variable `lxor` = `tcLmpi::lxor`
logical xor operation
- variable `bxor` = `tcLmpi::bxor`
bitwise xor operation
- variable `maxloc` = `tcLmpi::maxloc`
maximum and location operation
- variable `minloc` = `tcLmpi::minloc`
minimum and location operation
- variable `error` = `tcLmpi::error`
throw a Tcl error when a data conversion fails
- variable `abort` = `tcLmpi::abort`

- call `MPI_Abort()` when a data conversion fails*
 - variable `tozero` = `tclmpi::tozero`
silently assign zero for failed data conversions
 - variable `undefined` = `tclmpi::undefined`
constant to indicate an undefined number

7.1.1 Detailed Description

TclMPI package Tcl namespace

7.1.2 Function Documentation

7.1.2.1 `abort()`

```
proc tclmpi::abort (
    comm ,
    errorcode )
```

Terminates the MPI environment from Tcl

Parameters

<i>comm</i>	Tcl representation of an MPI communicator
<i>errorcode</i>	an integer that will be returned as exit code to the OS

This command makes a best attempt to abort all tasks sharing the communicator and exit with the provided error code. Only one task needs to call `tclmpi::abort`. This command terminates the program, so there can be no return value.

For implementation details see `TclMPI_Abort()`.

7.1.2.2 `allgather()`

```
proc tclmpi::allgather (
    data ,
    type ,
    comm )
```

Collects data from all processes on the communicator

Parameters

<i>data</i>	data to be distributed (Tcl data object)
<i>type</i>	data type to be used (string constant)
<i>comm</i>	Tcl representation of an MPI communicator

Returns

data that was collected or empty

This command collects data the provided list from all processes sharing the communicator. The data argument has to be present on all processes and has to be of the same length. The data resulting from the gather will be stored in the return value of the command for all processes. This function call is an implicit synchronization.

For implementation details see `TclMPI_Allgather()`.

7.1.2.3 allreduce()

```
proc tclmpi::allreduce (
    data ,
    type ,
    op ,
    comm )
```

Combines data from all processes and distributes the result back to them

Parameters

<i>data</i>	data to be reduced (Tcl data object)
<i>type</i>	data type to be used (string constant)
<i>op</i>	reduction operation (string constant)
<i>comm</i>	Tcl representation of an MPI communicator

Returns

data resulting from the reduction operation

This command performs a global reduction operation `op` on the provided data object across all processes participating in the communicator `comm`. If data is a list, then the reduction will be done across each respective entry of the same list index. The result is distributed to all processes and used as return value of the command. This command only supports the data types `tclmpi::int` and `tclmpi::double` and `tclmpi::intint` for operations `tclmpi::maxloc` and `tclmpi::minloc`. The following reduction operations are supported: `tclmpi::max` (maximum), `tclmpi::min` (minimum), `tclmpi::sum` (sum), `tclmpi::prod` (product), `tclmpi::land` (logical and), `tclmpi::band` (bitwise and), `tclmpi::lor` (logical or), `tclmpi::bor` (bitwise or), `tclmpi::lxor` (logical exclusive or), `tclmpi::bxor` (bitwise exclusive or), `tclmpi::maxloc` (max value and location), `tclmpi::minloc` (min value and location). This function call is an implicit synchronization.

For implementation details see `TclMPI_Allreduce()`.

7.1.2.4 barrier()

```
proc tclmpi::barrier (
    comm )
```

Synchronize MPI processes

Parameters

<i>comm</i>	Tcl representation of an MPI communicator
-------------	---

Blocks the caller until all processes sharing the communicator have called it; the call returns at any process only after **all** processes have entered the call and thus effectively synchronizes the processes. This function has no return value.

For implementation details see `TclMPI_Barrier()`.

7.1.2.5 bcast()

```
proc tclmpi::bcast (
    data ,
    type ,
    root ,
    comm )
```

Broadcasts data from one process to all processes on the communicator

Parameters

<i>data</i>	data to be broadcast (Tcl data object)
<i>type</i>	data type to be used (string constant)
<i>root</i>	rank of process that is providing the data (integer)
<i>comm</i>	Tcl representation of an MPI communicator

Returns

data that was broadcast

This command broadcasts the provided data object (list or single number or string) from the process with rank *root* on the communicator *comm* to all processes sharing the communicator. The data argument has to be present on all processes but will be ignored on all but the root process. The data resulting from the broadcast will be stored in the return value of the command on **all** processes. This is important when the data type is not `tclmpi::auto`, since using other data types may incur an irreversible conversion of the data elements. This function call is an implicit synchronization.

For implementation details see `TclMPI_Bcast()`.

7.1.2.6 comm_free()

```
proc tclmpi::comm_free (
    comm )
```

Deletes a dynamically created communicator and frees its resources

Parameters

<i>comm</i>	Tcl representation of an MPI communicator
-------------	---

This operation marks the MPI communicator associated with it Tcl representation *comm* for deallocation by the underlying MPI library. Any pending communications using this communicator will still complete normally.

For implementation details see `TclMPI_Comm_free()`.

7.1.2.7 comm_rank()

```
proc tclmpi::comm_rank (
    comm )
```

Returns the rank of the current process in an MPI communicator

Parameters

<i>comm</i>	Tcl representation of an MPI communicator
-------------	---

Returns

rank on the communicator (integer between 0 and size-1)

This function gives the rank of the process in the particular communicator. Many programs will be written with a manager-worker model, where one process (such as the rank-zero process) will play a supervisory role, and the other processes will serve as compute nodes. In this framework, [tclmpi::comm_size](#) and [tclmpi::comm_rank](#) are useful for determining the roles of the various processes of a communicator.

For implementation details see `TclMPI_Comm_rank()`.

7.1.2.8 comm_size()

```
proc tclmpi::comm_size (
    comm )
```

Returns the number of processes involved in an MPI communicator

Parameters

<i>comm</i>	Tcl representation of an MPI communicator
-------------	---

Returns

number of MPI processes on communicator

This function indicates the number of processes involved in a communicator. For [tclmpi::comm_world](#), it indicates the total number of processes available. This call is often used in combination with [tclmpi::comm_rank](#) to determine the amount of concurrency available for a specific library or program. [tclmpi::comm_rank](#) indicates the rank of the process that calls it in the range from 0...size-1, where size is the return value of [tclmpi::comm_size](#).

For implementation details see `TclMPI_Comm_size()`.

7.1.2.9 comm_split()

```
proc tclmpi::comm_split (
    comm ,
    color ,
    key )
```

Creates new communicators based on "color" and "key" flags

Parameters

<i>comm</i>	Tcl representation of an MPI communicator
<i>color</i>	subset assignment (non-negative integer or tclmpi::undefined)
<i>key</i>	relative rank assignment (integer)

Returns

Tcl representation of the newly created MPI communicator

This function partitions the group associated with *comm* into disjoint subgroups, one for each value of *color*. Each subgroup contains all processes of the same *color*. Within each subgroup, the processes are ranked in the order defined by the value of the argument *key*, with ties broken according to their rank in the old group. A new communicator is created for each subgroup and returned in *newcomm*. A process may supply the *color* value [tclmpi::undefined](#), in which case the function returns [tclmpi::comm_null](#). This is a collective call, but each process is permitted to provide different values for *color* and *key*.

The following example shows how to construct a communicator where the ranks are reversed in comparison to the world communicator.

```
set comm tclmpi::comm_world
set size [::tclmpi::comm_size $comm]
set key -[::tclmpi::comm_rank $comm]
set revcomm [::tclmpi::comm_split $comm 1 $key]
```

For implementation details see `TclMPI_Comm_split()`.

7.1.2.10 conv_get()

```
proc tclmpi::conv_get (
    handler )
```

Return a string constant naming the error handler for TclMPI data conversions

Returns

string constant for error handler

This function allows to query which error handler is currently active for Tcl data conversions inside TclMPI. For details on the error handlers, see [tclmpi::conv_set](#).

For implementation details see `TclMPI_Conv_get()`.

7.1.2.11 conv_set()

```
proc tclmpi::conv_set (
    handler )
```

Set the error handler for TclMPI data conversions

Parameters

<i>handler</i>	string constant for error handler
----------------	-----------------------------------

This function sets what action TcIMPI should take if a data conversion to [tclmpi::int](#) or [tclmpi::double](#) fails. When using data types other than [tclmpi::auto](#), the corresponding data needs to be converted from the internal Tcl representation to the selected native format. However, this does not always succeed for a variety of reasons. With this function TcIMPI allows the programmer to define how this is handled. There are currently three handlers available: [tclmpi::error](#) (the default setting), [tclmpi::abort](#), and [tclmpi::tozero](#). For [tclmpi::error](#) a Tcl error is raised that can be intercepted with catch and TcIMPI immediately returns to the calling function. For [tclmpi::abort](#) an error message is written directly to the screen and parallel execution on the current communicator is terminated via `MPI_Abort()`. For [tclmpi::tozero](#) the error is silently ignored and the data element set to zero. This command has no return value.

For implementation details see `TcIMPI_Conv_set()`.

7.1.2.12 `finalize()`

```
proc tclmpi::finalize ( )
```

Shut down the MPI environment from Tcl

This command closes the MPI environment and cleans up all MPI states. All processes must call this routine before exiting. Calling this function before calling [tclmpi::init](#) is an error. After calling this function, no more TcIMPI commands including [tclmpi::finalize](#) and [tclmpi::init](#) may be used. This command takes no arguments and has no return value.

For implementation details see `TcIMPI_Finalize()`.

7.1.2.13 `finalized()`

```
proc tclmpi::finalized ( )
```

Check if MPI environment was finalized from Tcl

Returns

boolean value of whether MPI has been shut down

This command checks if [tclmpi::finalize](#) has already been called or whether the MPI environment has been shut down otherwise. Since initializing MPI multiple times is an error, you can call this function to determine whether you need to call [tclmpi::finalize](#) and whether it is (still) allowed to call [tclmpi::init](#) in your Tcl script. This command takes no arguments.

For implementation details see `TcIMPI_Finalized()`.

7.1.2.14 `gather()`

```
proc tclmpi::gather (
    data ,
    type ,
    root ,
    comm )
```

Collects data from all processes on the communicator

Parameters

<i>data</i>	data to be distributed (Tcl data object)
<i>type</i>	data type to be used (string constant)
<i>root</i>	rank of process that will receive the data (integer)
<i>comm</i>	Tcl representation of an MPI communicator

Returns

data that was collected or empty

This command collects data the provided list from the process with rank `root` on the communicator `comm` to all processes sharing the communicator. The data argument has to be present on all processes and has to be of the same length. The data resulting from the gather will be stored in the return value of the command on the root process. This function call is an implicit synchronization. This procedure is the reverse operation of [tclmpi::scatter](#).

For implementation details see `TclMPI_Gather()`.

7.1.2.15 init()

```
proc tclmpi::init ( )
```

Initialize the MPI environment from Tcl

This command initializes the MPI environment. Needs to be called before any other TclMPI commands. MPI can be initialized at most once, so calling [tclmpi::init](#) multiple times is an error. Like in the C bindings for MPI, [tclmpi::init](#) will scan the argument vector, the global variable `$argv`, for any MPI implementation specific flags and will remove them. The global variable `$argc` will be adjusted accordingly. This command takes no arguments and has no return value.

For implementation details see `TclMPI_Init()`.

7.1.2.16 initialized()

```
proc tclmpi::initialized ( )
```

Check if MPI environment is initialized from Tcl

Returns

boolean value of whether MPI has been initialized

This command checks if [tclmpi::init](#) has already been called or whether the MPI environment has been set up otherwise. Since initializing MPI multiple times is an error, you can call this function to determine whether you need to call [tclmpi::init](#) in your Tcl script. This command takes no arguments.

For implementation details see `TclMPI_Initialized()`.

7.1.2.17 irecv()

```
proc tclmpi::irecv (
    type ,
    source ,
    tag ,
    comm )
```

Initiate a non-blocking receive

Parameters

<i>type</i>	data type to be used (string constant)
<i>source</i>	rank of sending process or tclmpi::any_source
<i>tag</i>	message identification tag or tclmpi::any_tag
<i>comm</i>	Tcl representation of an MPI communicator

Returns

Tcl representation of generated MPI request

This procedure provides a non-blocking receive operation, i.e. it returns **immediately**. The call does not return any data but a request handle of the form `tclmpi::req#`, with # being a unique integer number. This request handle is best stored in a variable and needs to be passed to a [tclmpi::wait](#) call to wait for completion of the receive and pass the data to the calling code as return value of the wait call. The type argument has to match that of the corresponding send command. Instead of a specific source rank, the constant [tclmpi::any_source](#) can be used and similarly [tclmpi::any_tag](#) as tag, to not select on source rank or tag, respectively.

For implementation details see `TclMPI_Irecv()`.

7.1.2.18 isend()

```
proc tclmpi::isend (
    data ,
    type ,
    dest ,
    tag ,
    comm )
```

Perform a non-blocking send

Parameters

<i>data</i>	data to be sent (Tcl data object)
<i>type</i>	data type to be used (string constant)
<i>dest</i>	rank of destination process (non-negative integer)
<i>tag</i>	message identification tag (integer)
<i>comm</i>	Tcl representation of an MPI communicator

Returns

Tcl representation of generated MPI request

This function performs a regular **non-blocking** send to process rank `dest` on communicator `comm`. The choice of data type determines how data is being sent and thus unlike in the C-bindings the corresponding receive has to use the same data type. As a non-blocking call, the function will return immediately. The return value is a string representing the generated MPI request and it can be passed to a call to [tclmpi::wait](#) in order to wait for its completion and release all reserved storage associated with the request.

For implementation details see `TclMPI_Isend()`.

7.1.2.19 probe()

```

proc tclmpi::probe (
    source ,
    tag ,
    comm ,
    status = {} )

```

Blocking test for a message

Parameters

<i>source</i>	rank of sending process or tclmpi::any_source
<i>tag</i>	message identification tag or tclmpi::any_tag
<i>comm</i>	Tcl representation of an MPI communicator
<i>status</i>	variable name for status array (string)

Returns

empty

This function allows to check for an incoming message on the communicator `comm` without actually receiving it. Nevertheless, this call is blocking, i.e. it will not return unless there is actually a message pending that matches the requirements of source rank and message tag. Instead of a specific source rank, the constant [tclmpi::any_source](#) can be used and similarly [tclmpi::any_tag](#) as tag, to accept send requests from any rank or tag, respectively. The (optional) status argument would be the name of a variable in which status information about the message will be stored in the form of an array. This associative array has the entries MPI_SOURCE (rank of sender), MPI_TAG (tag of message), COUNT_CHAR (size of message in bytes), COUNT_INT (size of message in [tclmpi::int](#) units), COUNT_DOUBLE (size of message in [tclmpi::double](#) units).

For implementation details see `TclMPI_Probe()`.

7.1.2.20 recv()

```

proc tclmpi::recv (
    type ,
    source ,
    tag ,
    comm ,
    status = {} )

```

Perform a blocking receive

Parameters

<i>type</i>	data type to be used (string constant)
<i>source</i>	rank of sending process or tclmpi::any_source
<i>tag</i>	message identification tag or tclmpi::any_tag
<i>comm</i>	Tcl representation of an MPI communicator
<i>status</i>	variable name for status array (string)

Returns

the received data

This procedure provides a blocking receive operation, i.e. it only returns **after** the message is received in full. The received data will be passed as return value. The type argument has to match that of the corresponding send command. Instead of using a specific source rank, the constant `tcimpi::any_source` can be used and similarly `tcimpi::any_tag` as tag. This way the receive operation will not select a message based on source rank or tag, respectively. The (optional) status argument would be the name of a variable in which status information about the receive will be stored in the form of an array. The associative array has the entries MPI_SOURCE (rank of sender), MPI_TAG (tag of message), COUNT_CHAR (size of message in bytes), COUNT_INT (size of message in `tcimpi::int` units), COUNT_DOUBLE (size of message in `tcimpi::double` units).

For implementation details see `TcIMPI_Recv()`.

7.1.2.21 reduce()

```
proc tcimpi::reduce (
    data ,
    type ,
    op ,
    root ,
    comm )
```

Combines data from all processes on one process

Parameters

<i>data</i>	data to be reduced (Tcl data object)
<i>type</i>	data type to be used (string constant)
<i>op</i>	reduction operation (string constant)
<i>root</i>	rank of process that is receiving the result (integer)
<i>comm</i>	Tcl representation of an MPI communicator

Returns

data resulting from the reduction operation

This command performs a global reduction operation `op` on the provided data object across all processes participating in the communicator `comm`. If data is a list, then the reduction will be done across each respective entry of the same list index. The result is collect on the process with rank `root` and used as return value of the command. For all other processes the return value is empty. This command only supports the data types `tcimpi::int` and `tcimpi::double` and `tcimpi::intint` for operations `tcimpi::maxloc` and `tcimpi::minloc`. The following reduction operations are supported: `tcimpi::max` (maximum), `tcimpi::min` (minimum), `tcimpi::sum` (sum), `tcimpi::prod` (product), `tcimpi::land` (logical and), `tcimpi::band` (bitwise and), `tcimpi::lor` (logical or), `tcimpi::bor` (bitwise or), `tcimpi::lxor` (logical exclusive or), `tcimpi::bxor` (bitwise exclusive or), `tcimpi::maxloc` (max value and location), `tcimpi::minloc` (min value and location). This function call is an implicit synchronization.

For implementation details see `TcIMPI_Reduce()`.

7.1.2.22 scatter()

```
proc tclmpi::scatter (
    data ,
    type ,
    root ,
    comm )
```

Distributes data from one process to all processes on the communicator

Parameters

<i>data</i>	data to be distributed (Tcl data object)
<i>type</i>	data type to be used (string constant)
<i>root</i>	rank of process that is providing the data (integer)
<i>comm</i>	Tcl representation of an MPI communicator

Returns

data that was distributed

This command distributes the provided list of data from the process with rank *root* on the communicator *comm* to all processes sharing the communicator. The data argument has to be present on all processes but will be ignored on all but the root process. The data resulting from the scatter will be stored in the return value of the command. The data will be distributed evenly, so the length of the list has to be divisible by the number of processes on the communicator. This procedure is the reverse operation of [tclmpi::gather](#). This function call is an implicit synchronization.

For implementation details see `TclMPI_Scatter()`.

7.1.2.23 send()

```
proc tclmpi::send (
    data ,
    type ,
    dest ,
    tag ,
    comm )
```

Perform a blocking send

Parameters

<i>data</i>	data to be sent (Tcl data object)
<i>type</i>	data type to be used (string constant)
<i>dest</i>	rank of destination process (non-negative integer)
<i>tag</i>	message identification tag (integer)
<i>comm</i>	Tcl representation of an MPI communicator

This function performs a regular **blocking** send to process rank *dest* on communicator *comm*. The choice of data type determines how data is being sent and thus unlike in the C-bindings the corresponding receive has to use the

same data data type. As a blocking call, the function will only return when all data is sent. This function has no return value.

For implementation details see `TclMPI_Send()`.

7.1.2.24 wait()

```
proc tclmpi::wait (
    request ,
    status = {} )
```

Non-blocking test for a message

Parameters

<i>source</i>	rank of sending process or tclmpi::any_source
<i>tag</i>	message identification tag or tclmpi::any_tag
<i>comm</i>	Tcl representation of an MPI communicator
<i>status</i>	variable name for status array (string)

Returns

1 or 0 depending on whether a pending request was detected

This function allows to check for an incoming message on the communicator `comm` without actually receiving it. Unlike [tclmpi::probe](#), this call is non-blocking, i.e. it will return immediately and report whether there is a message pending or not in its return value (1 or 0, respectively). Instead of a specific source rank, the constant [tclmpi::any_source](#) can be used and similarly [tclmpi::any_tag](#) as tag, to test for send requests from any rank or tag, respectively. The (optional) status argument would be the name of a variable in which status information about the message will be stored in the form of an array. This associative array has the entries `MPI_SOURCE` (rank of sender), `MPI_TAG` (tag of message), `COUNT_CHAR` (size of message in bytes), `COUNT_INT` (size of message in [tclmpi::int](#) units), `COUNT_DOUBLE` (size of message in [tclmpi::double](#) units).

For implementation details see `TclMPI_lprobe()`. Wait for MPI request completion

Parameters

<i>request</i>	Tcl representation of an MPI request
<i>status</i>	variable name for status array (string)

Returns

empty or received data that was associated with the request

This function takes a communication request created by a non-blocking send or receive call ([tclmpi::isend](#) or [tclmpi::irecv](#)) and waits for its completion. In case of a send, it will merely wait until the matching communication is completed and any resources associated with the request will be released. If the request was generated by a non-blocking receive call, [tclmpi::wait](#) will hand the received data to the calling routine in its return value. The (optional) status argument would be the name of a variable in which the resulting status information will be stored in the form of an associative array. The associative array will have the entries `MPI_SOURCE` (rank of sender), `MPI_TAG` (tag of message), `COUNT_CHAR` (size of message in bytes), `COUNT_INT` (size of message in [tclmpi::int](#) units), `COUNT_DOUBLE` (size of message in [tclmpi::double](#) units).

For implementation details see `TclMPI_Wait()`.

7.1.2.25 waitall()

```
proc tclmpi::waitall (
    requests ,
    status = {} )
```

Wait for multiple MPI request completions

Parameters

<i>requests</i>	List of Tcl representations of an MPI request
<i>status</i>	variable name for array with list of statuses (string)

Returns

empty or list of received data that was associated with the request

This function takes a list communication requests created by non-blocking send or receive call ([tclmpi::isend](#) or [tclmpi::irecv](#)) and waits for the completion of all of them. In case of a send, it will merely wait until the matching communication is completed and any resources associated with the request will be released. If the request was generated by a non-blocking receive call, [tclmpi::wait](#) will hand the received data to the calling routine in its return value. The (optional) status argument would be the name of a variable in which the resulting status information will be stored in the form of an associative array. The associative array will have the entries MPI_SOURCE (rank of sender), MPI_TAG (tag of message), COUNT_CHAR (size of message in bytes), COUNT_INT (size of message in [tclmpi::int](#) units), COUNT_DOUBLE (size of message in [tclmpi::double](#) units) and the results will be stored as lists with the information in the same order as the list of requests.

This call is implemented in Tcl as a wrapper around [tclmpi::wait](#)

7.2 tclmpi_test Namespace Reference

Functions

- proc [test_format](#) (kind, cmd, result)
- proc [compare](#) (reflist, result)
- proc [ser_init](#) (args)
- proc [par_init](#) (args)
- proc [run_return](#) (cmd, retval)
- proc [run_error](#) (cmd, errmsg)
- proc [par_return](#) (cmd, retval, [comm=tclmpi::comm_world](#))
- proc [par_error](#) (cmd, retval, [comm=tclmpi::comm_world](#))
- proc [test_summary](#) (section)

Variables

- set [version](#)
version of the package
- variable [comm](#) = [tclmpi::comm_world](#)
shortcut for world communicator
- variable [master](#) = 0

- rank of MPI master process*
 - variable `rank` = 0
- rank of this MPI process on \$comm*
 - variable `size` = 1
- number of processes on \$comm*
 - variable `int` = `tcimpi::int`
- shortcut for `tcimpi::int` data type*
 - variable `intint` = `tcimpi::intint`
- shortcut for `tcimpi::intint` data type*
 - variable `maxloc` = `tcimpi::maxloc`
- shortcut for `tcimpi::maxloc` operator*
 - variable `minloc` = `tcimpi::minloc`
- shortcut for `tcimpi::minloc` operator*
 - variable `pass` = 0
- counter for successful tests*
 - variable `fail` = 0
- counter for failed tests*

7.2.1 Detailed Description

TcIMPI test harness implementation namespace

This namespace contains several Tcl procedures that are used to conduct unit tests on the TcIMPI package. For simplicity paths are hardcoded, so that this file must not be moved around and stay in the same directory as the individual tests, which in turn have to be in a subdirectory of the directory where the TcIMPI shared object and/or the tcimpish extended Tcl shell reside.

7.2.2 Function Documentation

7.2.2.1 `compare()`

```
proc tcimpi_test::compare (
    refflist ,
    result )
```

partial result and error message comparison

Parameters

<i>refflist</i>	list of strings that have to appear in the result
<i>result</i>	result string

Returns

1 if all refflist strings were found in result

This function does an inexact comparison of the reference data to the actual result. The reference is a list of strings, each of which has to be matched in a case insensitive string search. The function returns a 1 if all tests did match.

7.2.2.2 par_error()

```
proc tclmpi_test::par_error (
    cmd ,
    retval ,
    comm = tclmpi::comm_world )
```

run a parallel test that is expected to produce a Tcl error

Parameters

<i>cmd</i>	list of strings or lists with the commands to execute
<i>retval</i>	list of the expected error message(s) or return values
<i>comm</i>	communicator. defaults to world communicator

Returns

empty

This function executes the lists command lines passed in \$cmd in parallel each command taken from the list based on the rank of the individual MPI task on the communicator and intercepts its resulting error message or return value using the 'catch' command. It is then checked if one of the commands failed as expected and actual return value are then compared against the expected reference passed in the \$retval list with similar assignments to the individual ranks as the commands. If one of the strings does not match or all command unexpectedly succeeded failure is reported otherwise success.

7.2.2.3 par_init()

```
proc tclmpi_test::par_init (
    args )
```

init for parallel tests

Parameters

<i>args</i>	all parameters are ignored
-------------	----------------------------

Returns

empty

This function will perform an initialization of the parallel environment for subsequent parallel tests. It also initializes the global variables \$rank and \$size.

7.2.2.4 par_return()

```
proc tclmpi_test::par_return (
    cmd ,
```

```

    retval ,
    comm = tclmpi::comm_world )

```

run a parallel test that is expected to succeed

Parameters

<i>cmd</i>	list of strings or lists with the commands to execute
<i>retval</i>	list of the expected return values
<i>comm</i>	communicator. defaults to world communicator

Returns

empty

This function executes the lists command lines passed in \$cmd in parallel each command taken from the list based on the rank of the individual MPI task on the communicator and intercepts its resulting return value using the 'catch' command. The actual return value is then compared against the expected reference passed in the \$retval list, similarly assigned to the individual ranks as the commands. The result is compared on all ranks and if one of the commands failed or the actual return value is not equal to the expected one, failure is reported and both, expected and actual results are printed on one of the failing ranks. The error reporting expects that the MPI communicator remains usable after failure.

7.2.2.5 run_error()

```

proc tclmpi_test::run_error (
    cmd ,
    errmsg )

```

run a serial test that is expected to fail

Parameters

<i>cmd</i>	string or list with the command to execute
<i>errmsg</i>	expected error message contents

Returns

empty

This function executes the command line passed in \$cmd and intercepts its resulting error using the 'catch' command. The actual error message is then compared against the expected reference passed in \$errmsg. The test is passed if the two strings match, otherwise failure is reported and both the expected and actual error messages are printed. Also an unexpectedly successful execution is considered a failure and its result reported for reference.

7.2.2.6 run_return()

```

proc tclmpi_test::run_return (
    cmd ,
    retval )

```

run a serial test that is expected to succeed

Parameters

<i>cmd</i>	string or list with the command to execute
<i>retval</i>	expected return value contents

Returns

empty

This function executes the command line passed in \$cmd and intercepts its resulting return value using the 'catch' command. The actual return value is then compared against the expected reference passed in \$retval. The test is passed if the two strings match, otherwise failure is reported and both the expected and actual results are printed. Also an unexpectedly failure of the command is reported as failure and the resulting error message is reported for debugging.

7.2.2.7 ser_init()

```
proc tclmpi_test::ser_init (  
    args )
```

init for serial tests

Parameters

<i>args</i>	all parameters are ignored
-------------	----------------------------

Returns

empty

This function will perform a simple init test requesting the tclmpi package and matching it against the current version number. It will also initialize some commonly used global variables. If called from a parallel environment, it will only execute and produce output on the master process

7.2.2.8 test_format()

```
proc tclmpi_test::test_format (  
    kind ,  
    cmd ,  
    result )
```

format output

Parameters

<i>kind</i>	string representing the kind of test (max 11 chars).
<i>cmd</i>	string representing the command. will be truncated as needed.
<i>result</i>	string indicating the result (PASS or FAIL/reason)

Returns

the formatted string

This function will format a test summary message, so that it does not break the output on a regular terminal screen. The first column will be the total number of the test computed from the sum of passed and failed tests, followed by a string describing the test type, the command executed and a result string. The command string in the middle will be truncated as needed to not break the format.

7.2.2.9 test_summary()

```
proc tclmpi_test::test_summary (
    section )
```

print result summary

Parameters

<i>section</i>	number of the test section
----------------	----------------------------

Returns

empty

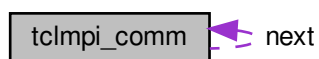
This function will print a nicely formatted summary of the tests. If executed in parallel only the master rank of the world communicator will produce output.

Chapter 8

Class Documentation

8.1 tclmpi_comm Struct Reference

Collaboration diagram for tclmpi_comm:



Public Attributes

- const char * [label](#)
- MPI_Comm [comm](#)
- int [valid](#)
- [tclmpi_comm_t](#) * [next](#)

8.1.1 Detailed Description

Linked list entry to map MPI communicators to strings.

8.1.2 Member Data Documentation

8.1.2.1 comm

```
MPI_Comm tclmpi_comm::comm
```

MPI communicator corresponding of this entry

8.1.2.2 label

```
const char* tclmpi_comm::label
```

String representing the communicator in Tcl

8.1.2.3 next

```
tclmpi_comm_t* tclmpi_comm::next
```

Pointer to next element in linked list

8.1.2.4 valid

```
int tclmpi_comm::valid
```

Non-zero if communicator is valid

The documentation for this struct was generated from the following file:

- `_tclmpi.c`

8.2 tclmpi_dblint Struct Reference

Public Attributes

- double `d`
- int `i`

8.2.1 Detailed Description

Represent a double/integer pair

8.2.2 Member Data Documentation

8.2.2.1 d

```
double tclmpi_dblint::d
```

double data value

8.2.2.2 i

```
int tclmpi_dblint::i
```

location data

The documentation for this struct was generated from the following file:

- `_tclmpi.c`

8.3 tclmpi_intint Struct Reference

Public Attributes

- int [i1](#)
- int [i2](#)

8.3.1 Detailed Description

Represent an integer/integer pair

8.3.2 Member Data Documentation

8.3.2.1 i1

```
int tclmpi_intint::i1
```

integer data value

8.3.2.2 i2

```
int tclmpi_intint::i2
```

location data

The documentation for this struct was generated from the following file:

- `_tclmpi.c`

8.4 tclmpi_req Struct Reference

Collaboration diagram for tclmpi_req:



Public Attributes

- const char * [label](#)
- void * [data](#)
- int [len](#)
- int [type](#)
- int [source](#)
- int [tag](#)
- MPI_Request * [req](#)
- MPI_Comm [comm](#)
- tclmpi_req_t * [next](#)

8.4.1 Detailed Description

Linked list entry to map MPI requests to "tclmpi::req%d" strings.

8.4.2 Member Data Documentation

8.4.2.1 comm

```
MPI_Comm tclmpi_req::comm
```

communicator for non-blocking receive

8.4.2.2 data

```
void* tclmpi_req::data
```

pointer to send or receive data buffer

8.4.2.3 label

```
const char* tclmpi_req::label
```

identifier of this request

8.4.2.4 len

```
int tclmpi_req::len
```

size of data block

8.4.2.5 next

```
tclmpi_req_t* tclmpi_req::next
```

pointer to next struct

8.4.2.6 req

```
MPI_Request* tclmpi_req::req
```

pointer MPI request handle generated by MPI

8.4.2.7 source

```
int tclmpi_req::source
```

source rank of non-blocking receive

8.4.2.8 tag

```
int tclmpi_req::tag
```

tag selector of non-blocking receive

8.4.2.9 type

```
int tclmpi_req::type
```

data type of send data

The documentation for this struct was generated from the following file:

- `_tclmpi.c`

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