Challenge Problems in Verification of MPI Programs

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Outline

1. Problem Statement
2. A Brief Tutorial on MPI
3. Challenge 1 (Deterministic): Parametric Verification of Ghost Cell Exchanges
4. Challenge 2 (Nondeterministic): Verification of Manager-Worker Codes

Message Passing Interface: Background

- MPI = "Message Passing Interface"
- a standardized library for writing message-passing parallel programs
  - in C, C++, or Fortran
- **MPI: A Message Passing Interface Standard**
  - v1.0 (1994), . . . , v4.1 (2023)
  - `https://www.mpi-forum.org`
- universal in scientific/HPC computing
  - weather prediction, climate change
  - design of aircraft, engines, buildings
  - genome sequencing
  - prediction of protein structure
  - certifying nuclear reactor safety
  - monitoring/simulation of nuclear weapons
  - prediction of seismic activity

Univ. Delaware Verified Software Lab
Aurora supercomputer
Argonne National Laboratory, USA

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  - a process can obtain its unique ID ("rank")
    - by branching on rank, each process can execute different code

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- What I can do now: small scope verification
  - using model checking and symbolic execution techniques
  - place (small) bounds on `nprocs`, input sizes
  - verify assertions, deadlock-freedom, functional equivalence
  - verify a function conforms to its contracts
  - tools: MPI-Spin, TASS, CIVL Model Checker — `https://civl.dev`

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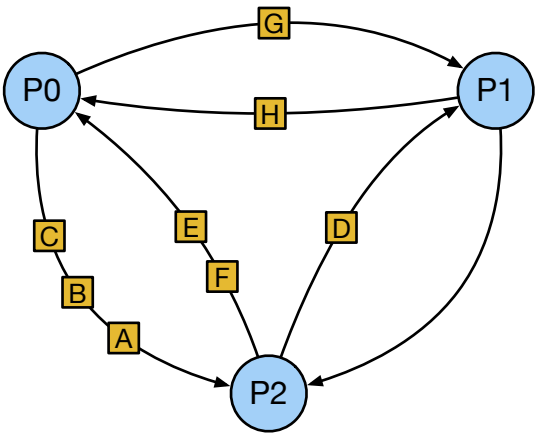
- What I really want
  - verification for arbitrary number of processes
  - with minimal manual effort (annotations, hints, proof assistant interactions...)

Hello, world

```
#include<stdio.h>
#include<mpi.h>
int main() {
  int rank, nprocs;
  MPI_Init(NULL, NULL);
  MPI_Comm_size(MPI_COMM_WORLD, &nprocs); // get the number of procs
  MPI_Comm_rank(MPI_COMM_WORLD, &rank); // get this proc's PID
  printf("Hello from MPI process %d of %d!\n", rank, nprocs);
  fflush(stdout);
  MPI_Finalize();
}
```

```
> mpicc -o hello.exec hello.c
> mpiexec -n 4 hello.exec
Hello from MPI process 0 of 4!
Hello from MPI process 3 of 4!
Hello from MPI process 1 of 4!
Hello from MPI process 2 of 4!
>
```

Message channels: conceptual framework



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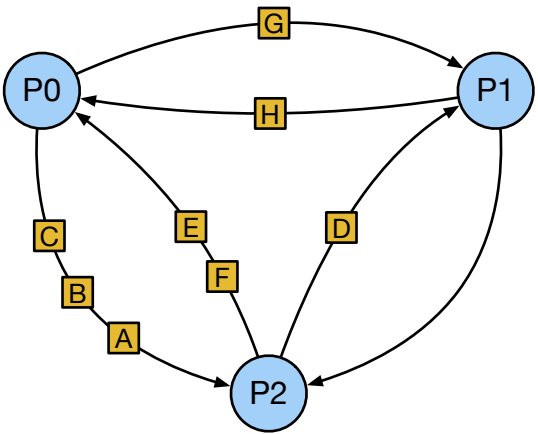

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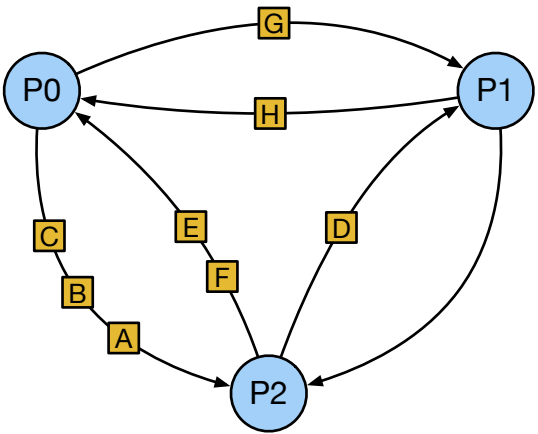

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  - including from proc to itself (rarely used)

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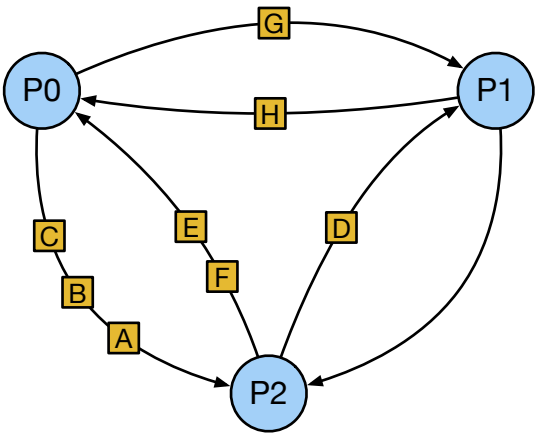

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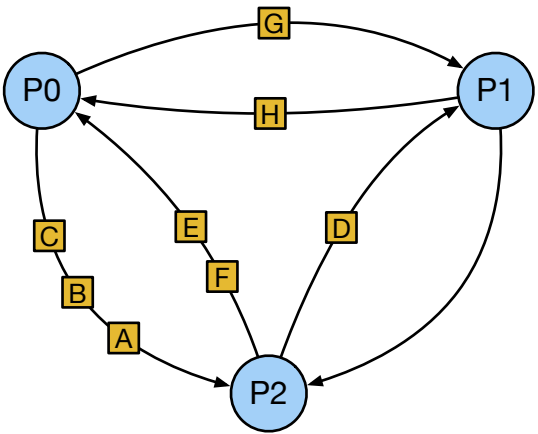

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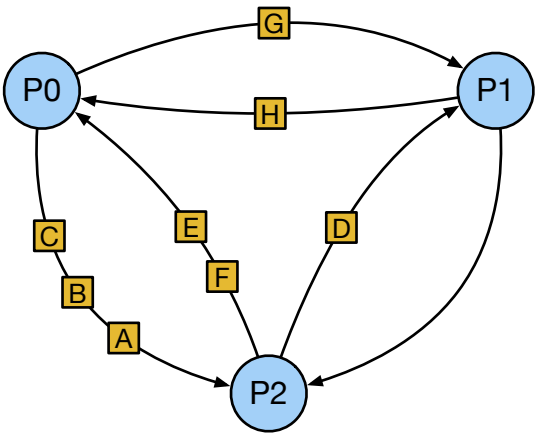

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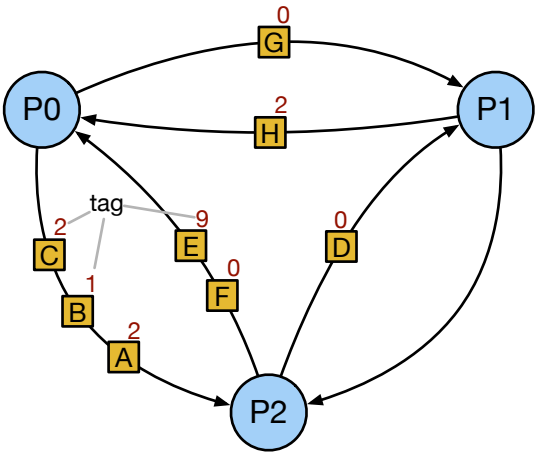
  - messages from one communicator are never picked up by an operation from a different communicator
- between any 2 procs, there is a p2p message channel
  - including from proc to itself (rarely used)
- `send` enqueues message
- `recv` dequeues message
- mostly a FIFO queue

Tags



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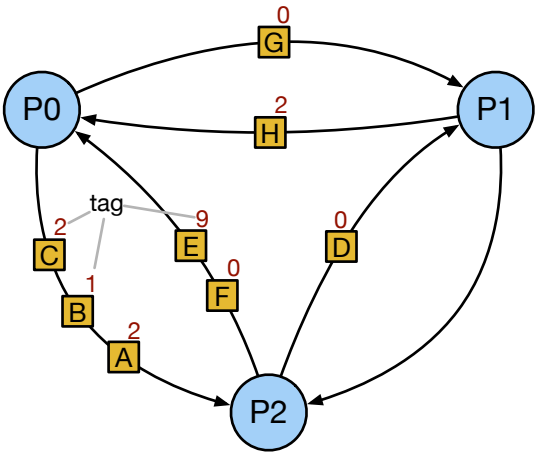

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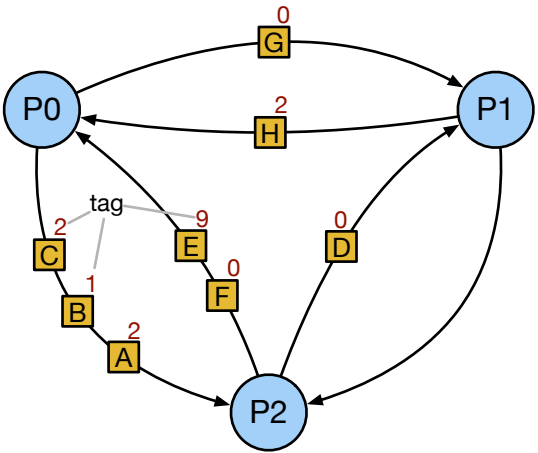

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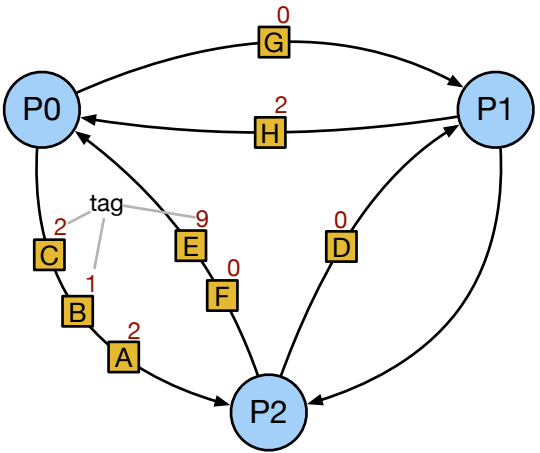

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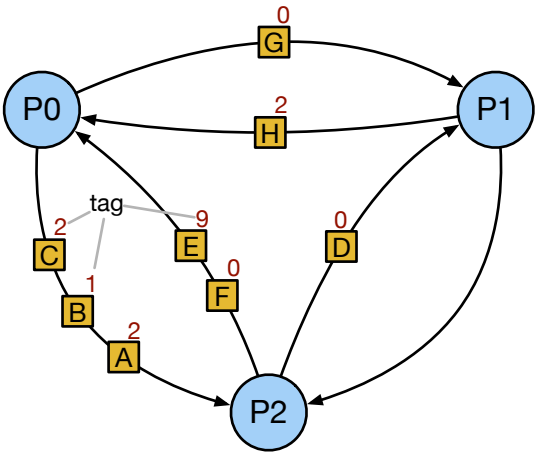

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- if P2 issues recv from P0 with tag 1
  - P2 will receive message B
  - the first (oldest) message in queue with matching tag
- if P2 issues recv from P0 with "any tag"
  - P2 will receive message A

MPI_Send

```
MPI_Send(buf, count, datatype, dest, tag, comm)
```

`buf`	address of send buffer (`void*`)
`count`	number of elements in buffer (`int`)
`datatype`	data type of elements in buffer (`MPI_Datatype`)
`dest`	rank of destination process (`int`)
`tag`	integer to attach to message envelope (`int`)
`comm`	communicator (`MPI_Comm`)

MPI_Recv

```
MPI_Recv(buf, count, datatype, source, tag, comm, status)
```

`buf`	address of receive buffer (`void*`)
`count`	number of elements in buffer (`int`)
`datatype`	data type of elements in buffer (`MPI_Datatype`)
`source`	rank of source process (`int`)
`tag`	tag of message to receive (`int`)
`comm`	communicator (`MPI_Comm`)
`status`	pointer to status object (`MPI_Status*`)

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  - otherwise, undefined behavior

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- `count` must be at least as large as count of incoming message
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- `status`: object to store envelope information on received message
  - source, tag, count
  - if you don't need it, use `MPI_STATUS_IGNORE`

Example: cyclic exchange: `cycle1.c`

Processes attempt to exchange data in a cycle (ring).
Everyone first sends to their right, then receives from their left.

```
#include<stdio.h>
#include<mpi.h>
int main() {
  int nprocs, rank;
  MPI_Init(NULL, NULL);
  MPI_Comm_rank(MPI_COMM_WORLD, &rank);
  MPI_Comm_size(MPI_COMM_WORLD, &nprocs);
  const int right = (rank + 1)%nprocs, left = (rank + nprocs - 1)%nprocs;
  int rbuf, sbuf = 100 + rank;
  MPI_Send(&sbuf, 1, MPI_INT, right, 0, MPI_COMM_WORLD);
  MPI_Recv(&rbuf, 1, MPI_INT, left, 0, MPI_COMM_WORLD, MPI_STATUS_IGNORE);
  printf("Proc %d: received %d\n", rank, rbuf);
  MPI_Finalize();
}
```

Synchronization and potential deadlock

- `cycle1.c` has a problem
- a send operation may block until a matching receive is called
  - buffer space is finite
- each send may be buffered or may be forced to synchronize
- a correct program will behave correctly regardless of how these decisions are made
- to correct the cyclic exchange. . .
  - good: make even processes send first; odd processes receive first

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- a correct program will behave correctly regardless of how these decisions are made
- to correct the cyclic exchange...
  - good: make even processes send first; odd processes receive first
  - better... this situation is so common, MPI provides a function to deal with it
  - `MPI_Sendrecv` combines one send and one receive operation into a single command
  - both operations execute concurrently

MPI_Sendrecv

```
MPI_Sendrecv(sbuf, scount, stype, dest, stag,
             rbuf, rcount, rtype, source, rtag,
             comm, status)
```

`sbuf`	address of send buffer (`void*`)
`scount`	number of elements in send buffer (`int`)
`stype`	data type of elements in sbuf (`MPI_Datatype`)
`dest`	rank of destination process (`int`)
`stag`	integer to attach to message envelope (`int`)
`rbuf`	address of receive buffer (`void*`)
`rcount`	length of receive buffer (`int`)
`rtype`	data type of elements to be received (`MPI_Datatype`)
`source`	rank of sending process (`int`)
`rtag`	tag of message to receive (`int`)
`comm`	communicator (`MPI_Comm`)
`status`	pointer to status object for receive (`MPI_Status*`)

Correct cyclic exchange using MPI_Sendrecv: cycle.c

```
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#include<mpi.h>
int main() {
  int nprocs, rank;
  MPI_Init(NULL, NULL);
  MPI_Comm_rank(MPI_COMM_WORLD, &rank);
  MPI_Comm_size(MPI_COMM_WORLD, &nprocs);
  const int right = (rank + 1)%nprocs, left = (rank + nprocs - 1)%nprocs;
  int rbuf, sbuf = 100 + rank;
  MPI_Sendrecv(&sbuf, 1, MPI_INT, right, 0, &rbuf, 1, MPI_INT, left, 0,
               MPI_COMM_WORLD, MPI_STATUS_IGNORE);
  printf("Proc %d: received %d\n", rank, rbuf);
  MPI_Finalize();
}
```
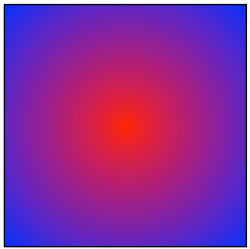

2-d Diffusion

- a rectangular metal plate
  - initially $100°$
  - temperature on perimeter kept at $0°$
  - over time, heat diffuses out of plate
- $u = u(x, y, t)$ temperature function
- 2d diffusion equation

$$\frac{\partial u}{\partial t} = \alpha \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right)$$



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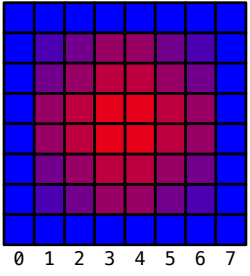
- discretization

```
u_new[i][j] =  u[i][j]
  + k*(u[i+1][j] + u[i-1][j]
    + u[i][j+1] + u[i][j-1] - 4*u[i][j]);
```



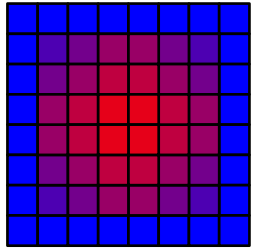
diffusion2d.c: sequential code (excerpt)

```
int nx, ny;                /* dimensions of the plate */
double k;                  /* constant controlling rate of diffusion */
int nstep;                 /* number of time steps */
double ** u, ** u_new;     /* two copies of temperature function */
...
void update() {
  for (int i = 1; i < nx - 1; i++)
    for (int j = 1; j < ny - 1; j++)
      u_new[i][j] = u[i][j] +
        k*(u[i+1][j] + u[i-1][j] + u[i][j+1] + u[i][j-1] - 4*u[i][j]);
  double ** const tmp = u_new; u_new = u; u = tmp;
}

int main() {
  for (int i = 1; i <= nstep; i++) {
    update();
    write();
  }
}
```

Parallelization of diffusion2d by column distribution

- block distribute the columns of `u` among the processes
- each process updates its columns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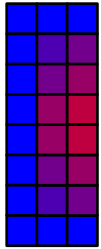
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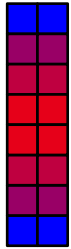
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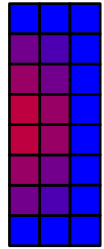
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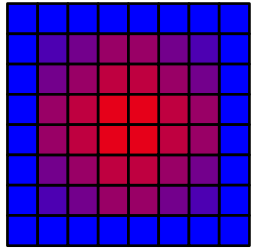
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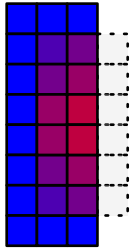
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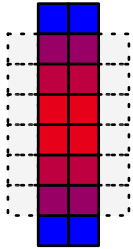
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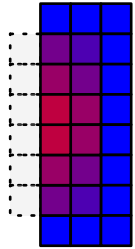
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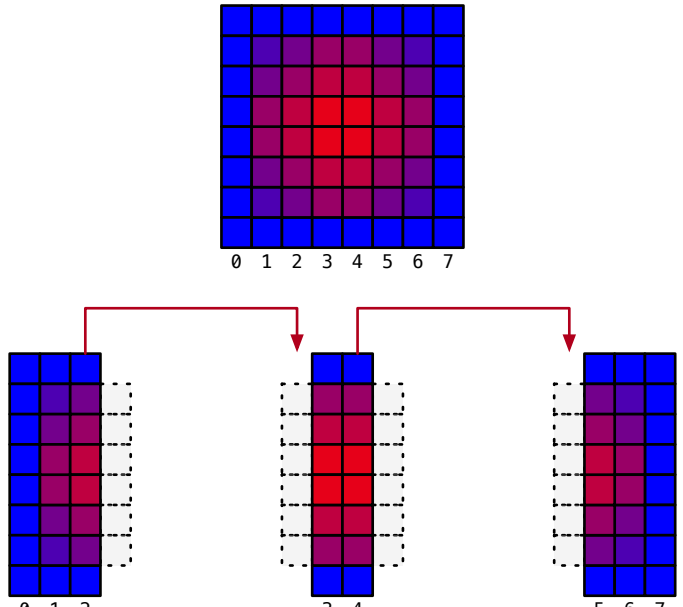
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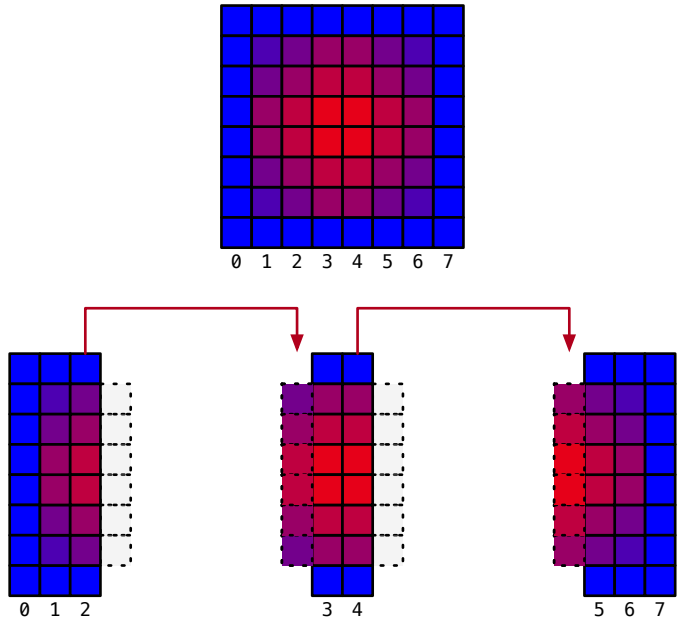
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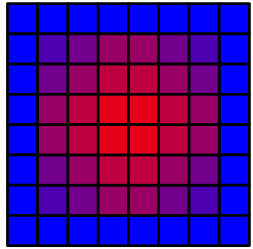
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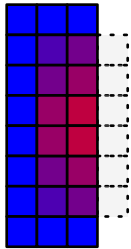
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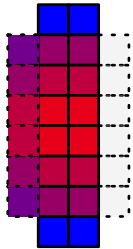
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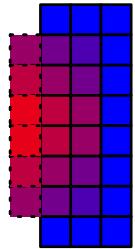
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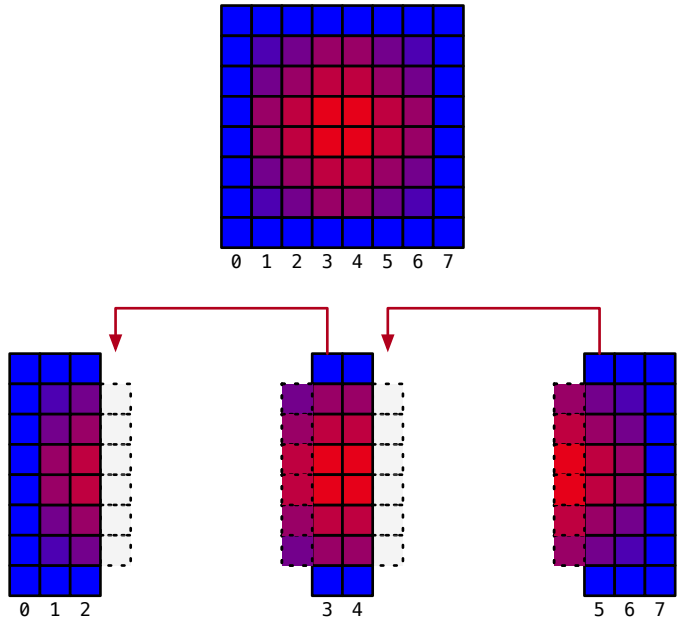
0 1 2 3 4 5 6 7
0 1 2
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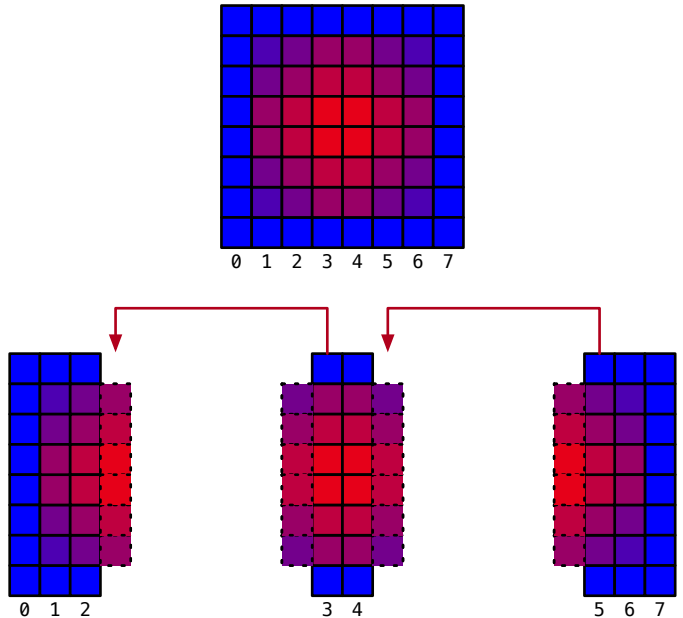
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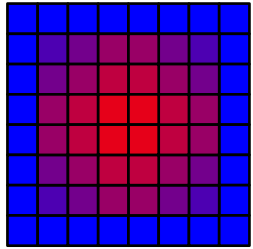
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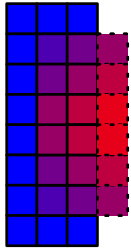
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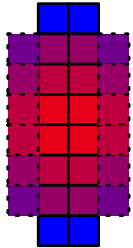
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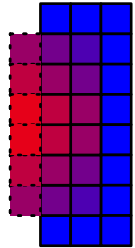

5 6 7

diffusion2d_mpi.c (excerpt)

```
static void exchange_ghost_cells() {
  MPI_Sendrecv(u[1], ny, MPI_DOUBLE, left, 0,
               u[nxl+1], ny, MPI_DOUBLE, right, 0, MPI_COMM_WORLD, MPI_STATUS_IGNORE);
  MPI_Sendrecv(u[nxl], ny, MPI_DOUBLE, right, 0,
               u[0], ny, MPI_DOUBLE, left, 0, MPI_COMM_WORLD, MPI_STATUS_IGNORE);
}

void update() {
  for (int i = start; i <= stop; i++)
    for (int j = 1; j < ny-1; j++)
      u_new[i][j] = u[i][j] + k*(u[i+1][j] + u[i-1][j] + u[i][j+1] + u[i][j-1] - 4*u[i][j]);
  double ** const tmp = u_new; u_new = u; u = tmp;
}

int main() {
  for (int i = 1; i <= nstep; i++) {
    exchange_ghost_cells();
    update();
    write();
  }
}
```

See diffusion2d2.mp4.

Challenge 1

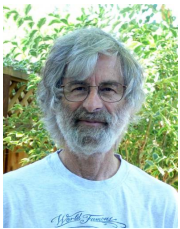
- construct mechanized proof that `diffusion2d_mpi.c` is functionally correct
  - for any `nx`, `ny`, `nprocs`
- correctness is specified by
  - functional equivalence with `diffusion2d.c`, or
  - any other reasonable way (e.g., a contract)

An attempt to verify a simple cyclic exchanger

- Ziqing Luo & I tried to verify a simple message-passing program performing a repeated cyclic exchange
- *Second International Workshop on Software Correctness for HPC Applications* (2018)

```
1 int rank, nprocs, nsteps;
2 double rbuf, sbuf;
3 #define  LEFT(pid) ((pid)>0 ? (pid)-1 : nprocs-1)
4 #define RIGHT(pid) ((pid)<nprocs-1 ? (pid)+1 : 0)
5 ...
6 void exchange() {
7     int t = 0;
8     while (t < nsteps) {
9         send(&sbuf, RIGHT(rank));
10        recv(&rbuf, LEFT(rank));
11        sbuf = rbuf;
12        t++;
13    }
14 }
```

An attempt to verify a simple cyclic exchanger



Owicki and I and most everyone else thought that the Owicki-Gries method was a great improvement over Ashcroft's method because it used the program text to decompose the proof. I've since come to realize that this was a mistake. It's better to write a global invariant. . . . Ashcroft got it right.

— Leslie Lamport

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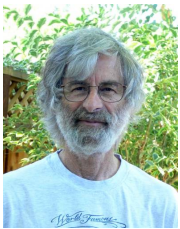

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- we attempted a mechanized proof of C code using a global invariant
  - ACSL, Frama-C+WP: verify invariant preserved by each atomic step of a process
- variables represented as arrays of length `nprocs`
- extra array for control location of each process
- message buffers represented as arrays
- invariant relates all of above

Frama-C + WP Verification of Cyclic Exchange: Excerpt

```
/*@ axiomatic OracleSpec {
  @   logic double oracle(int t, int i);
  @   axiom oracle_ax: \forall int t,i; t > 0 ==>
  @           oracle(t-1, LEFT(i)) == oracle(t, i);
  @ }
 */

//@ . . .
//@ predicate inv1 = \forall int i; 0 <= i < nprocs ==>
                size[i] == 1 ==> chan[i] == oracle(sc[i]-1, i)

//@ . . .
//@ predicate inv2 = \forall int i; 0 <= i < nprocs ==>
                      rc[i] == sc[LEFT(i)] - size[LEFT(i)];
//@ . . .

#define inv (. . . inv1 && inv2 && . . .)
```

Frama-C + WP Verification of Cyclic Exchange: Summary

- 54 lines of ACSL annotations for 17 lines of C code
- all verification conditions but 1 discharged with Why3, Alt-Ergo, CVC4
- one VC implying deadlock-freedom could not be proved by any automated prover
  - we could prove it using CVC4 for `nprocs` ≤ 200
  - we could prove it by hand
  - Sebastiaan Joosten proved it using Isabelle ($\sim$150 lines)

```
#define NPROCSB 20
#define LEFT(rank) ((rank) > 0 ? (rank) - 1 : nprocs - 1)
//@ ghost int sc[NPROCSB], rc[NPROCSB], sizes[NPROCSB];
int nprocs, nsteps;
/* note that inv0 and inv5 is not needed for proving the deadlock-freedom condition */
/*@ axiomatic FDL {
  @
  @ predicate inv1 = \forall integer i; 0 <= i < nprocs ==> 0 <= sizes[i] <= 1;
  @ predicate inv2 = \forall integer i; 0 <= i < nprocs ==> 0 <= sc[i] <= nsteps;
  @ predicate inv3 = \forall integer i; 0 <= i < nprocs ==> 0 <= rc[i] <= nsteps;
  @ predicate inv4 = \forall integer i; 0 <= i < nprocs ==> rc[i]==sc[LEFT(i)]-sizes[LEFT(i)];
  @ predicate inv6 = \forall integer i; 0 <= i < nprocs ==> (sc[i]-rc[i]==0) || (sc[i]-rc[i]==1);
  @ predicate fdl = \exists integer i; 0 <= i < nprocs && ((sc[i]-rc[i]==0 && sizes[i]==0) || (sc[i]-rc[i]==1 && sizes[LEFT(i)]==1));
  @
  @  lemma bounded_free_of_deadlock : inv1 && inv2 && inv3 && inv4 && inv6 && 0<nprocs<=NPROCSB
  @                                   ==> fdl;
  @ } */
```

Related Work

ParTypes

- *A Type Discipline for Message Passing Parallel Programs*
  - Vasconcelos, Martins, López, Yoshida
  - ACM ToPLaS 2022
- based on **session types**
- user specifies a communication protocol in a simple language
  - this defines a type
- an algorithm checks that each process conforms to the protocol (has the specified type)
- works for deterministic programs like `diffusion2d_mpi.c`
- verifies deadlock-freedom, termination for any number of processes
- does not say anything about the computation

Nondeterminism

- all examples so far are deterministic
  - for a given input...
  - any two executions are equivalent
    - one can be obtained from the other by repeatedly transposing adjacent commuting transitions
  - for any process p: sequence of process states of p is the same for any execution
  - executions only differ by how actions from processes are interleaved
  - this is known *a priori* because of the subset of MPI used
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    - in particular: each receive statement specifies its source
- many algorithms in scientific computing can be expressed deterministically
- but some algorithms require a process to receive from any source
- MPI provides a way to do this
  - the `source` argument to `MPI_Recv` may be `MPI_ANY_SOURCE`
  - a "wildcard" receive

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- Example (based on example from **Using MPI**): matrix multiplication: compute AB
  - manager has A; every worker gets a complete copy of B
  - a task: compute one row of AB

Manager-Worker pseudocode

```
count := 0;
while count < P − 1 do
    send ⟨count + 1, A[count]⟩ to count + 1;
    count := count + 1;
end while
i := 0;
while i < N do
    ⟨tag, T⟩ := recv(any(source));
    C[tag − 1] := T;
    if count < N then
        send ⟨count + 1, A[count]⟩ to source;
        count := count + 1;
    end if
    i := i + 1;
end while
```

Manager

```
while true do
    ⟨tag, in⟩ := recv(0);
    out := in ∗ B;
    send ⟨tag, out⟩ to 0;
end while
```

Worker

matmat_mpi.c: matrix multiplication, manager-worker, excerpt

```
void manager() { ...
  // Broadcast entire matrix B to all workers...
  MPI_Bcast(&b[0][0], L*M, MPI_DOUBLE, 0, comm);
  // Send one task to each worker, unless you run out of tasks...
  for (count = 0; count < nprocs-1 && count < N; count++)
    MPI_Send(&a[count][0], L, MPI_DOUBLE, count+1, count+1, comm);
  // Receive result, insert into C, send the next task, repeat...
  for (int i = 0; i < N; i++) {
    MPI_Recv(tmp, M, MPI_DOUBLE, MPI_ANY_SOURCE, MPI_ANY_TAG, comm, &status);
    for (int j = 0; j < M; j++)
      c[status.MPI_TAG-1][j] = tmp[j];
    worker_counts[status.MPI_SOURCE]++;
    if (count < N) {
      MPI_Send(&a[count][0], L, MPI_DOUBLE, status.MPI_SOURCE, count+1, comm);
      count++;
    }
  }
  // send termination signals (tag=0) to all workers...
}
```

Challenge 2

- Construct a mechanized proof that for any
  - $L, M, N \geq 1$,
  - $N \times L$ matrix A and $L \times M$ matrix B,
  - `nprocs` ≥ 2
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A first step...

- a "LaTeX proof"
- construction of a global invariant
- invariant under each atomic code block

Variables used to model state of `matmat_mpi.c`

W = set of process ranks of workers

1. u_j ($j \in W$) : buffered messages from manager to worker j
2. v_j ($j \in W$) : buffered messages from worker j to manager
3. all variables in manager
   - `count`, `i`, ...
4. auxiliary data for manager
   - Solved (set of int): set of tasks solved, initially empty
   - Out (set of int): set of tasks sent out but solution not yet received
5. for each j, all variables in worker j
   - `tag`, `in`, ...
6. auxiliary data for worker j
   - InWorker[j] (set of int): set of tasks that worker j is currently working on
     - cardinality at most 1

Auxiliary definitions used to express invariant of `matmat_mpi.c`

$$\mathsf{ToWorker}[j] = \bigcup_{\langle t,V\rangle \in u[j]} \{t-1\}$$

$$\mathsf{ToManager}[j] = \bigcup_{\langle t,T\rangle \in v[j]} \{t-1\}$$

$$\mathsf{InWorker} = \bigcup_{j \in W} \mathsf{InWorker}[j]$$

$$\mathsf{ToWorker} = \bigcup_{j \in W} \mathsf{ToWorker}[j]$$

$$\mathsf{ToManager} = \bigcup_{j \in W} \mathsf{ToManager}[j]$$

The "core invariant" of `matmat`

Let disjoint be the assertion that says the $3(P-1)$ sets InWorker$[*]$, ToWorker$[*]$, ToManager$[*]$ are pairwise disjoint.

Let Φ denote the assertion

$$
\begin{aligned}
& \mathsf{Out} \cap \mathsf{Solved} = \emptyset \\
\wedge\ & \mathsf{Out} \cup \mathsf{Solved} = \{0, \ldots, \mathit{count} - 1\} \\
\wedge\ & \mathsf{Out} = \mathsf{InWorker} \cup \mathsf{ToWorker} \cup \mathsf{ToManager} \\
\wedge\ & \mathsf{disjoint} \\
\wedge\ & (\forall j \in \mathsf{Solved}.\ C[j] = A[j] * B) \\
\wedge\ & (\forall j \in W.\ \forall \langle t, V \rangle \in u[j].\ V = A[t-1]) \\
\wedge\ & (\forall j \in W.\ \forall \langle t, T \rangle \in v[j].\ T = A[t-1] * B).
\end{aligned}
$$

Claim: Φ is invariant under each atomic block of `matmat`.

$\{\Phi\}$
$count := 0;\ \mathsf{Out} := \emptyset;\ \mathsf{Solved} = \emptyset;$
$\{0 \leq count \leq P-1 \wedge \mathsf{Solved} = \emptyset \wedge \Phi\}$
while $count < P-1$ **do**
  $\{0 \leq count < P-1 \wedge \mathsf{Solved} = \emptyset \wedge \Phi\}$
  send $\langle count+1, A[count]\rangle$ **to** $count+1;\ \mathsf{Out} := \mathsf{Out} \cup \{count\};\ count := count+1;$
  $\{0 \leq count \leq P-1 \wedge \mathsf{Solved} = \emptyset \wedge \Phi\}$
end while
$\{count = P-1 \wedge \mathsf{Solved} = \emptyset \wedge \Phi\}$
$i := 0;$
$\{0 \leq i \leq N \wedge |\mathsf{Solved}| = i \wedge count = \min\{i+P-1, N\} \wedge \Phi\}$
while $i < N$ **do**
  $\{0 \leq i < N \wedge |\mathsf{Solved}| = i \wedge count = \min\{i+P-1, N\} \wedge \Phi\}$
  $\langle tag, T\rangle :=$ **recv**(**any**(*source*));
  $C[tag-1] := T;\ \mathsf{Solved} := \mathsf{Solved} \cup \{tag-1\};\ \mathsf{Out} := \mathsf{Out} \setminus \{tag-1\};$
  $\{0 \leq i < N \wedge |\mathsf{Solved}| = i+1 \wedge count = \min\{i+P-1, N\} \wedge \Phi\}$
  if $count < N$ **then**
    $\{count < N \wedge 0 \leq i < N \wedge |\mathsf{Solved}| = i+1 \wedge count = i+P-1 \wedge \Phi\}$
    send $\langle count+1, A[count]\rangle$ **to** *source*; $\mathsf{Out} := \mathsf{Out} \cup \{count\};\ count := count+1;$
  end if
  $\{0 \leq i < N \wedge |\mathsf{Solved}| = i+1 \wedge count = \min\{i+P, N\} \wedge \Phi\}$
  $i := i+1;$
  $\{0 \leq i \leq N \wedge |\mathsf{Solved}| = i \wedge count = \min\{i+P-1, N\} \wedge \Phi\}$
end while
$\{|\mathsf{Solved}| = N \wedge \Phi\}$

Verification of Manager-Worker

- I believe this proof is correct
- how can it be formally attached to the source code and mechanized?
- how can the annotation burden and effort be minimized?
- what tools can help?