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MATLAB HPC Mentors

June 25, 2020

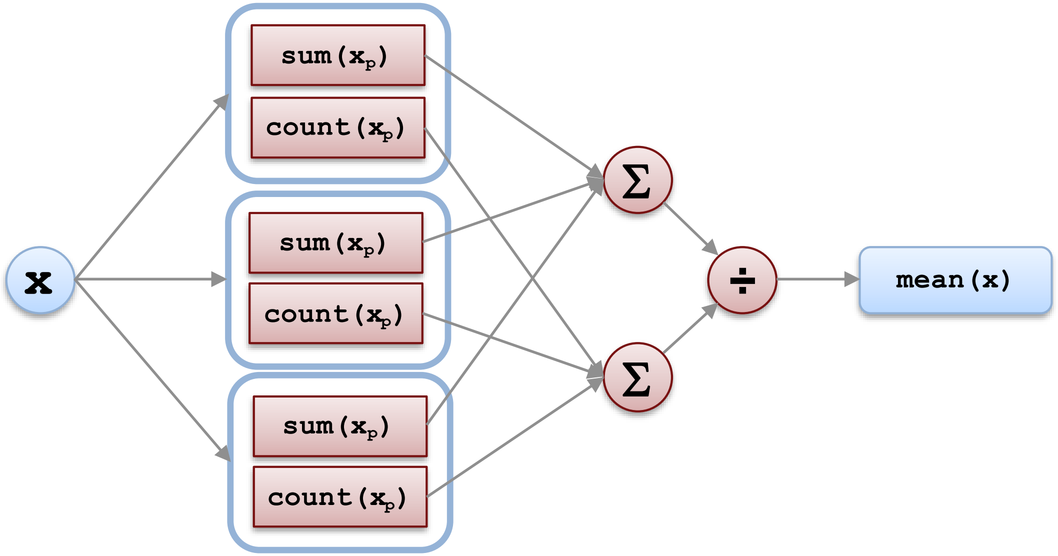
Host: **Nicholas Ide**

Guest Speakers: **Ben Tordoff** & **Oli Tissot**, Parallel Computing Development

Quick Updates

- No meeting in July or August – enjoy the summer, stay healthy!
- If you have issues with recent SSH and MATLAB Parallel Server, let me know.
  - Have been a few reports
  - Members of the community have found temporary solutions

Distributed Arrays: techniques and best practices for handling very large calculations



Ben Tordoff & Oli Tissot,
Parallel Computing Development

Agenda

- ➔ What are distributed arrays?
- What can you do with distributed arrays?
- Building a distributed array
- Advanced manoeuvres
- Debugging methods and tips

Remote arrays in MATLAB

Rule: take the calculation to where the data is

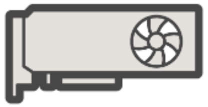
Normal array – calculation happens in main memory:

```
x = rand(...)

x_norm = (x - mean(x)) ./ std(x)
```

Remote arrays in MATLAB

Rule: take the calculation to where the data is

gpuArray – all calculation happens on the GPU:

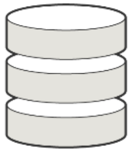


```
x = gpuArray(...)

x_norm = (x - mean(x)) ./ std(x)
```

distributed – calculation is spread across the memory of a cluster:

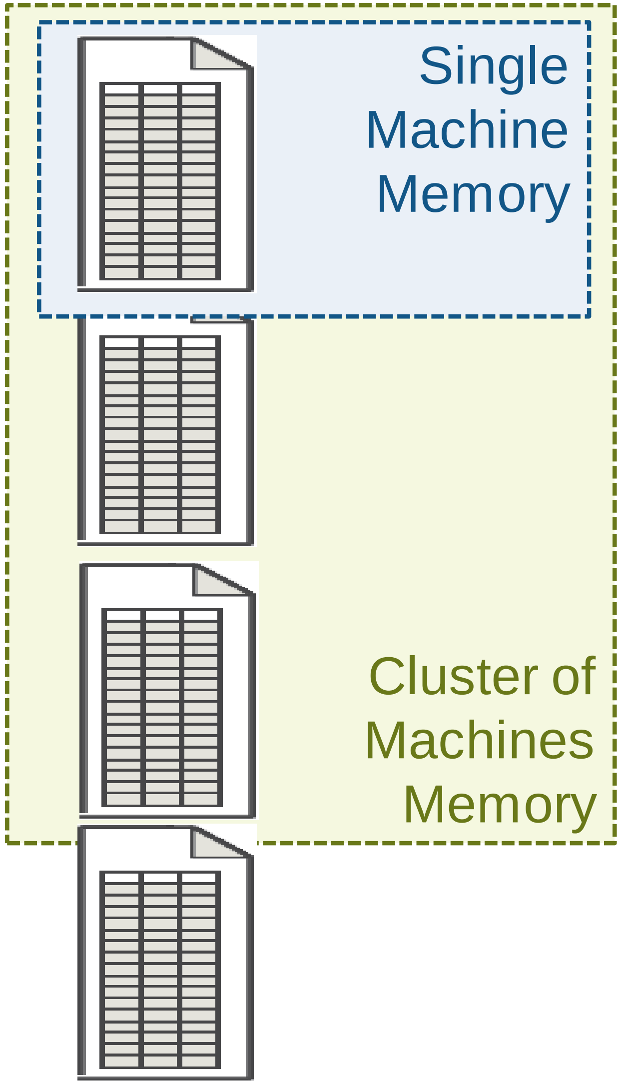
```
x = distributed(...)

x_norm = (x - mean(x)) ./ std(x)
```

tall – calculation is performed by stepping through files:



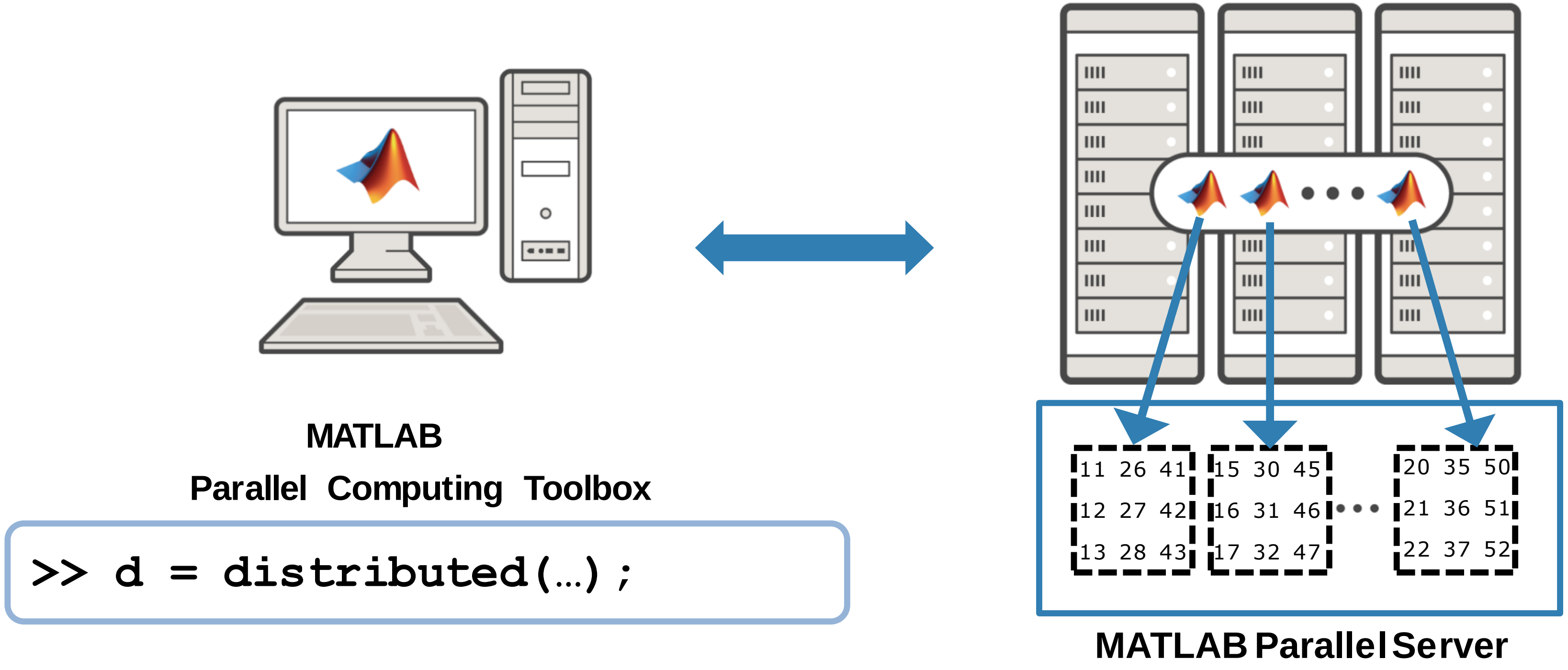
```
x = tall(...)

x_norm = (x - mean(x)) ./ std(x)
```

When should I reach for distributed?



- If your data fits in memory, just use MATLAB normally
- If it won't fit on one machine, maybe it can be split across the combined memory of a cluster of machines? Use `distributed` arrays
- If it won't fit in the combined memory of a cluster of machines then use `tall` arrays

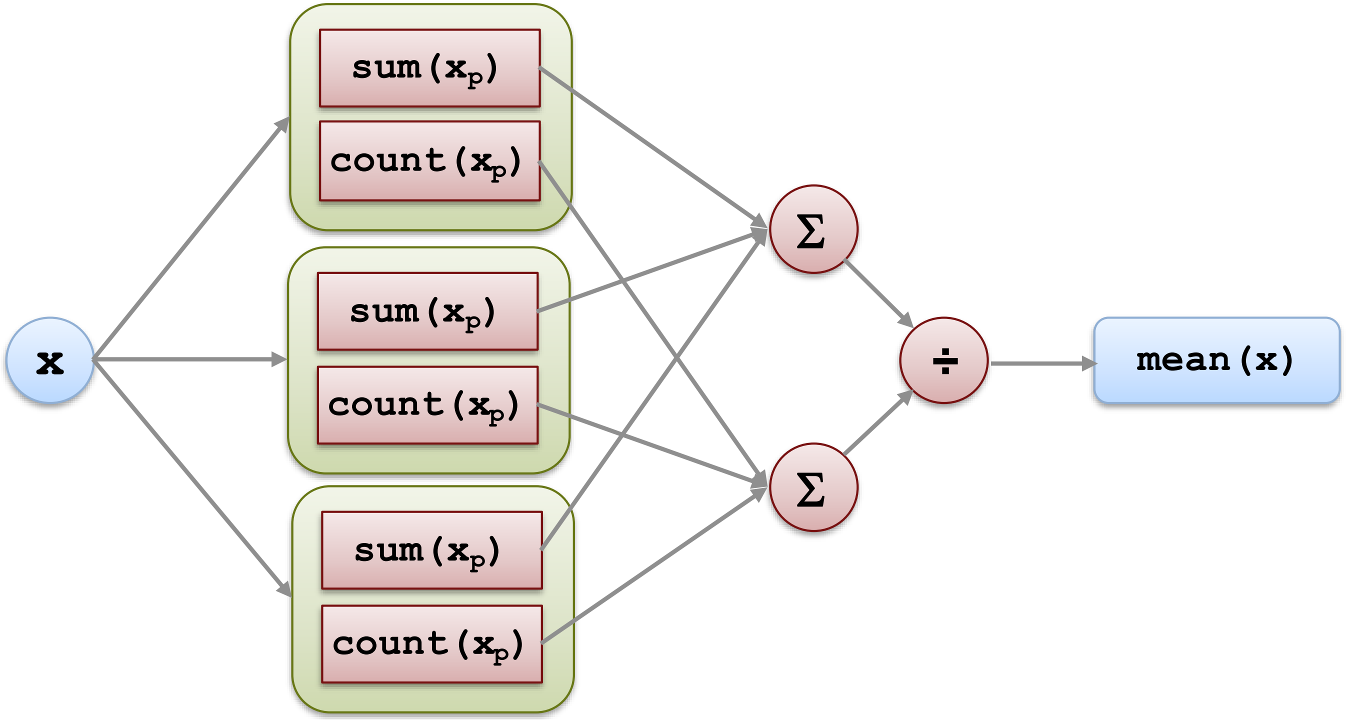
Using distributed arrays



- Use the memory of multiple machines as though it was your own
- Client sees a “normal” MATLAB variable
- Work happens on cluster

Distributed Algorithms

```
>> m = mean(d);
```



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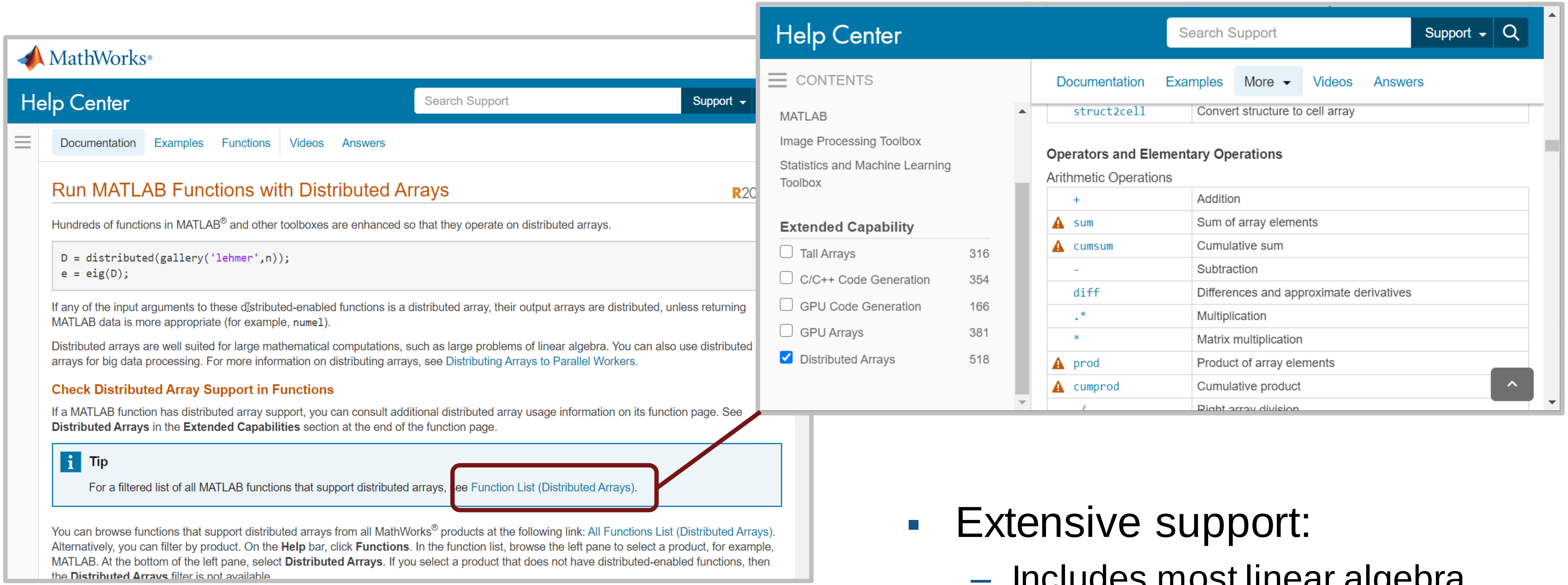
What can you do with distributed arrays?

Distributed array functions



- Extensive support:
  - Includes most linear algebra
  - Scale up mathematical operations

[Run MATLAB functions with distributed arrays]

What can you do with distributed arrays?

- >500 functions supported (as of R2020a)
- support for dense and sparse linear algebra
- support for numerics (double, single, logical, etc.)
- support for datetimes, durations, categoricals, tables, …

- focus is on data preparation and large system solve

What can you do with distributed arrays?

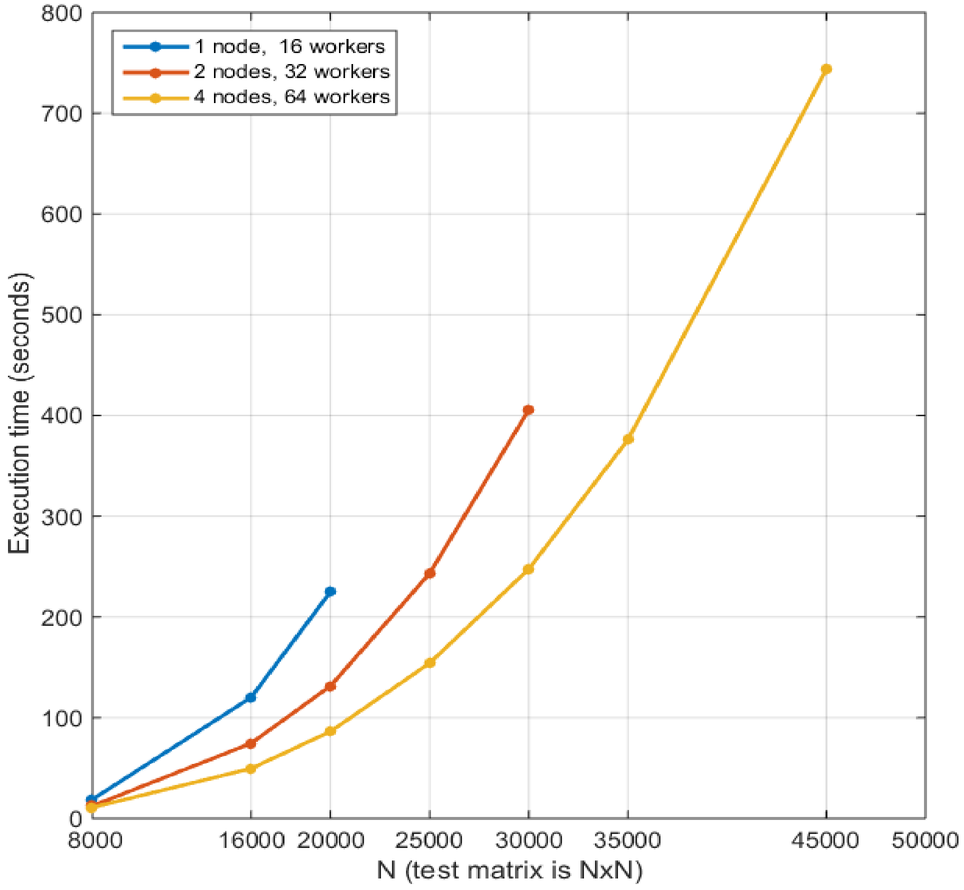
Code written for distributed arrays looks like normal MATLAB code

```
% Create / read distributed data
A = distributed(...)

% Same code as for in-memory
b = sum(A,2);
x1 = A\b; % direct solution
x2 = pcg(A, b); % iterative solution

% Bring back from cluster
[x1,x2] = gather(x1, x2);
```

Processing quite big data

Multiplication of 2 NxN matrices

```
>> C = A * B
```



N	Execution time (seconds)		
	1 node, 16 workers	2 nodes, 32 workers	4 nodes, 64 workers
8000	19	13	11
16000	120	75	50
20000	225	132	86
25000	-	243	154
30000	-	406	248
35000	-	-	376
45000	-	-	743
50000	-	-	-

Processor: Intel Xeon E5-class v2
16 cores, 60 GB RAM per compute node, 10 Gb Ethernet

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Building a distributed array

There are four main ways to build a distributed array:

1. Create from in-memory data
2. Build functions
3. Read from datastore
4. Construct from local parts

Building a distributed array: from in-memory

```
>> x = gallery("poisson",10000);
>> dx = distributed(x); % Data sent to workers
```

- All data is sent from client to workers
- Useful for debugging before scaling up
- Useful for data that is close to filling local memory (i.e. can be created but not operated on due to fill-in etc.)

Building a distributed array: build functions

```
>> dx = distributed.ones(1e9,100);
>> dx = distributed.rand(1e9,100);
>> dx = distributed.speye(1e9);
>> dx = distributed.sprand(1e9,1e9,1e-8);
... etc.
```

- No data is sent from client to workers
- Useful for creating test data and examples

Building a distributed array: build from datastore

Datastore:

- Simple interface for data in multiple files/folders
- Presents data a piece at a time
- Access pieces in serial (desktop) or in parallel (cluster)
- Back-ends for tabular text, images, databases and more
- Data always stacked vertically

```
>> ds = datastore("data/*.csv")
>> preview(ds)
    Rows      Cols      Vals
    _____     _____     _____

        1         1         4
        2         1        -1
    10001         1        -1
        :         :         :
        :         :         :
```

Building a distributed array: build from datastore

Read datastore into distributed

- each worker reads its own part of the data
- data is distributed vertically (workers have blocks of rows)

```
>> dt = distributed(ds); % distributed table of [Rows, Cols, Vals]
>> d = sparse(dt.Rows, dt.Cols, dt.Vals);

>> size(d)
ans = 100000000  100000000

>> nnz(d)
ans = 499960000
```

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Writing your own algorithms

SPMD let's you craft parallel algorithms:

- Inside SPMD `distributed` -> `codistributed`
- `getLocalPart` extracts the data for this worker
- Use `gop` to reduce across workers (binary tree)
- Use `gcat` to concatenate results across workers

```
>> d = distributed(...)
>> spmd
       S = sum(getLocalPart(d)),"all"); % Sum values on this worker
       totalSum = gop(@plus, S); % Add results across all workers
   end
```

Writing your own algorithms

SPMD let's you craft parallel algorithms:

- MPI-like `labSend`, `labReceive`, `labSendReceive` for low level communication
- `labindex` for working out which worker you are

```
>> d = distributed(...)
>> spmd
       mydata = getLocalPart(d);
       % Cycle data to the right (wrapping round on last worker)
       prevWorker = mod(labindex-2, numlabs)+1; % worker to the left
       nextWorker = mod(labindex, numlabs)+1; % worker to the right
       mydata = labSendReceive(nextWorker, prevWorker, mydata)
   end
```

Modifying the data distribution

SPMD also gives control over distribution:

- `redistribute` for changing the distribution of an existing array
- `codistributorXX` for creating new (co)distributed arrays

```
>> d = distributed.ones(1e5); % Default is 1D distribution in dim 2
>> spmd
       % Switch to having whole rows per worker
       d2 = redistribute(d, codistributor1d(1));
       % Use a custom (uneven) distribution of the data
       partition = 1e4 * [1 2 3 4];
       d3 = redistribute(d, codistributor1d(1, partition));
       % Switch to block-cyclic
       d4 = redistribute(d, codistributor2dbc());
   end
```

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Debugging

Some rules of thumb:

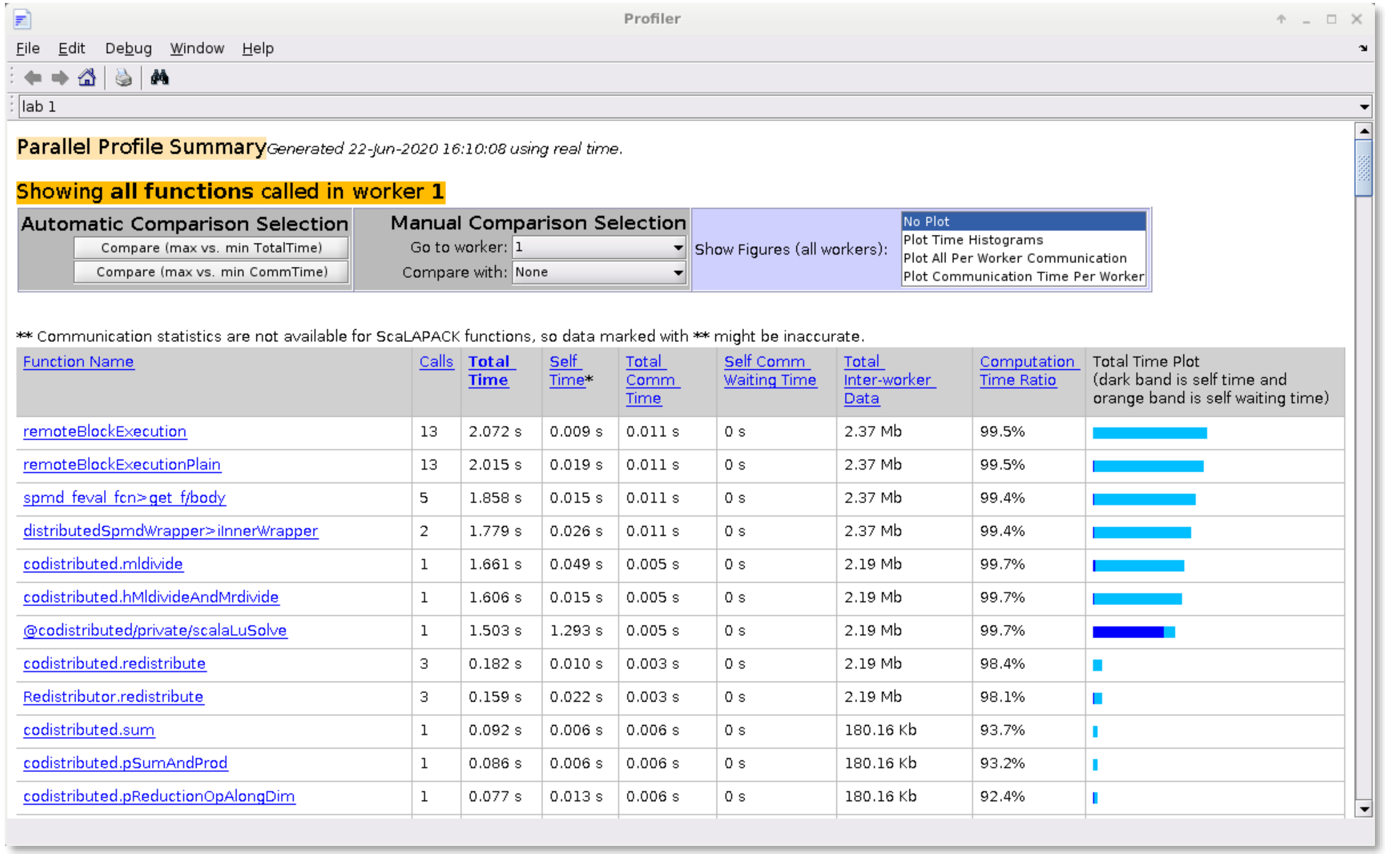
- Start with “local” pool and small data
  - faster iteration time
  - proves correctness
- Use pre-built algorithms if you can
- If writing your own, prefer higher-level gop, gcat over labSend/Receive
  - It’s easy to create mismatched communications with labSend/Receive!
  - Using unique tags for each communication helps to spot stray messages
  - Keeping computation and communication code separate helps in debugging both
- Run for a few different sizes to understand how duration scales with size
- Think about where your data lives – minimize transmission of files across networks

Debugging

Use parallel profiler (mpiprofiler):

- Shows what code ran, how much data transferred and allows comparison between workers (spot uneven loading)

```
>> mpiprofiler on
>> % Lots of parallel code ...
>> mpiprofview
```



Function Name	Calls	Total Time	Self Time*	Total Comm Time	Self Comm Waiting Time	Total Inter-worker Data	Computation Time Ratio	Total Time Plot (dark band is self time and orange band is self waiting time)
remoteBlockExecution	13	2.072 s	0.009 s	0.011 s	0 s	2.37 Mb	99.5%	
remoteBlockExecutionPlain	13	2.015 s	0.019 s	0.011 s	0 s	2.37 Mb	99.5%	
spmd_feval_fcn>get_f/body	5	1.858 s	0.015 s	0.011 s	0 s	2.37 Mb	99.4%	
distributedSpmdWrapper>iInnerWrapper	2	1.779 s	0.026 s	0.011 s	0 s	2.37 Mb	99.4%	
codistributed.mldivide	1	1.661 s	0.049 s	0.005 s	0 s	2.19 Mb	99.7%	
codistributed.hMldivideAndMrdivide	1	1.606 s	0.015 s	0.005 s	0 s	2.19 Mb	99.7%	
@codistributed/private/scalaLuSolve	1	1.503 s	1.293 s	0.005 s	0 s	2.19 Mb	99.7%	
codistributed.redistribute	3	0.182 s	0.010 s	0.003 s	0 s	2.19 Mb	98.4%	
Redistributor.redistribute	3	0.159 s	0.022 s	0.003 s	0 s	2.19 Mb	98.1%	
codistributed.sum	1	0.092 s	0.006 s	0.006 s	0 s	180.16 Kb	93.7%	
codistributed.pSumAndProd	1	0.086 s	0.006 s	0.006 s	0 s	180.16 Kb	93.2%	
codistributed.pReductionOpAlongDim	1	0.077 s	0.013 s	0.006 s	0 s	180.16 Kb	92.4%	

Debugging

Use spmd or parfevalonall to interact with workers and see local state

```
>> spmd, d, end

Lab 1: This worker stores d(:,1:1667).
          LocalPart: [10000x1667 double]
      Codistributor: [1x1 codistributor1d]

Lab 2: This worker stores d(:,1668:3334).
          LocalPart: [10000x1667 double]
      Codistributor: [1x1 codistributor1d]

Lab 3:
   etc.
```

Questions