

## Introduction



### Why use MATLAB for HPC?

- Familiar environment
- Portability
- Rapid prototyping
- License conservation
- Computational speed
- Lots of available packages and code



#### **MDCS** introduction

- MATLAB Distributed Computing Server (MDCS) is built over the message parsing interface (MPI) to allow scaling of Parallel Computing Toolbox (PCT) enabled codes
- Workers need only the MDCS worker license (provided by SNIC)
- Workers inherit all toolbox licenses from the submitting process
- Regular MATLAB license + PCT license is only needed during job submission
- PCT constructs scale seamlessly. I.e. same code can be used locally and on the cluster
- Code can be prototyped on local machine and then used on a HPC cluster to scale in computational power and memory footprint



#### MATLAB@NSC

- Available using ThinLinc and through terminal
- Integrated with the queueing system
- Distributes work on workers in a parallel-pool
- Up to 700 workers
- Larger memory and more cores
- Arrays can be distributed over all workers
- Can run applications Interactively or as Batch jobs



#### Desktop or Console?

- For full MATLAB interface ThinLinc is recommended
- If only the ability to send in scripts is needed, the console can suffice
- The ThinLinc client is for most users preferable (available at www.cendio.com/thinlinc/download)



# Setting up



#### **Command Window**

New to MATLAB? See resources for Getting Started.

>> configCluster

>> % Set ProjectName and WallTime before submitting jobs to AURORA

```
>> c = parcluster;
```

```
>> c.AdditionalProperties.ProjectName = 'project-name';
```

```
>> c.AdditionalProperties.WallTime = '01:00:00';
```

```
>> c.saveProfile
```

fx >>



#### **Command Window**

fx >>

New to MATLAB? See resources for Getting Started.

```
>> configCluster
```

```
>> % Set ProjectName and WallTime before submitting jobs to AURORA
>> c = parcluster;
>> c.AdditionalProperties.ProjectName = 'project-name';
>> c.AdditionalProperties.WallTime = '01:00:00';
>> c.saveProfile
>> c.AdditionalProperties.WallTime='00:10:00';
>> c.AdditionalProperties.ProjectName='aurora-test';
```

Older Installations used: configCluster ClusterInfo.setProjectName('name-of-proj') ClusterInfo.setWallTime('00:10:00')



Command Window						
New to MATLAB? See resources for <u>Getting Started</u> .						
>> configCluster						
>	<pre>&gt;&gt; % Set ProjectName and WallTime before submitting jobs to AURORA &gt;&gt; c = parcluster; &gt;&gt; c.AdditionalProperties.ProjectName = 'project-name'; &gt;&gt; c.AdditionalProperties.WallTime = '01:00:00'; &gt;&gt; c.saveProfile</pre>					
<pre>&gt;&gt; c=parcluster; &gt;&gt; c.AdditionalProperties.WallTime='00:10:00'; &gt;&gt; c.AdditionalProperties.ProjectName='aurora-test'; &gt;&gt; !projinfo (Counting the number of core hours used since 2017-10-06/00:00:00 until now.)</pre>						
Project User	Used[h]	Current allocation [h/month]				
aurora-test anfo hukebuck jhein marcosscc raymond	66.94 22.21 15.13 0.03 0.37 29.20	10000				
snic2016-1-146	0.00	5000				
snic2017-1-126 hukebuck	0.09 0.09	5000				
snic2017-4-9	0.00	5000				



Command Window							
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	snic2017-1-126 hukebuck	0.09 0.09	5000				
	snic2017-4-9	0.00	5000				
	<pre>&gt;&gt;&gt; c.AdditionalProperties ans =  <u>AdditionalProperties</u> with properties:  AdditionalSubmitArgs: '' DebugMessagesTurnedOn: 0 EmailAddress: '' MemUsage: '' DebugMesagesTurnedOn: 0</pre>						
	ProcsPerNode: 0 ProjectName: 'aurora-test' QueueName: '' RequestExclusiveNode: '' Reservation: ''						
fx	UseIdentityFile: 1 WallTime: '00:10:00'						

Older Installations used:

setArch setClusterHost setDataParallelism setDebugMessagesTurnedOn setDiskSpace setEmailAddress setGpusPerNode setMemUsage setNameSpace setPrivateKeyFile setPrivateKeyFileHasPassPhrase setProcsPerNode setProjectName setQueueName setRequireExclusiveNode setReservation setSshPort setUseGpu setUserDefinedOptions setUserNameOnCluster setWallTime



# **Basic concepts**



#### Workflows

•

Local host

All workers are running on the local host



#### Workflows

• Interactive



All workers are running on a remote host, controlled by the user process more or less directly





Jobs are dispatched to workers on one or more nodes, each with its o wn job id in SLURM. Note that each job has its own master worker



#### How do I start a parallel pool?

- parpool(n)
  - starts a parallel pool of n workers
- j = batch('script1','Pool',8)
  - starts a pool of 8 workers and runs the script script1 on those workers



#### How do I share code with workers?

- Workers Access Files Directly
- Pass Data to and from Worker Sessions
- Pass MATLAB Code for Startup and Finish



#### **Workers Access Files Directly**

- The workers all have access to the same drives on the network, they can access the necessary files that reside on these shared resources.
- Using the job's AdditionalPaths property
- Putting the path command in any of the appropriate startup files for the worker

'AdditionalPaths' — A string or cell array of strings that defines paths to be added to the MATLAB search path of the workers before the script or function executes.

matlabroot\toolbox\local\startup.m
matlabroot\toolbox\distcomp\user\jobStartup.m
matlabroot\toolbox\distcomp\user\taskStartup.m



#### Pass Data to and from Worker Sessions

- **InputArguments** Contains the input data you specified when creating the task. This data gets passed into the function when the worker performs its evaluation.
- **OutputArguments** Property of each task contains the results of the function's evaluation.
- JobData Property of the job object. Contains data that gets sent to every worker that evaluates tasks for that job. The data is passed to a worker only once per job.
- AttachedFiles Property of the job object. A cell array in which you manually specify all the folders and files that get sent to the workers. On the worker, the files are installed and the entries specified in the property are added to the search path of the worker session.
- AutoAttachFiles Property of the job object. A logical value to specify that you want MATLAB to perform an analysis on the task functions in the job and on manually attached files to determine which code files are necessary for the workers, and to automatically send those files to the workers.

The supported code file formats for automatic attachment are MATLAB files (.m extension), P-code files (.p), and MEX-files (.mex). Note that AutoAttachFiles does not include data files for your job; use the AttachedFiles property to explicitly transfer these files to the workers.



#### **Pass MATLAB Code for Startup and Finish**

- As in a session of MATLAB, a worker session executes its startup.m file each time it starts. You can place the startup.m file in any folder on the worker's MATLAB search path, such as toolbox/distcomp/user.
- These additional files can initialize and clean up a worker session as it begins or completes evaluations of tasks for a job:



#### Pass MATLAB Code for Startup and Finish

- **jobStartup.m** automatically executes on a worker when the worker runs its first task of a job.
- **taskStartup.m** automatically executes on a worker each time the worker begins evaluation of a task.
- **poolStartup.m** automatically executes on a worker each time the worker is included in a newly started parallel pool.
- **taskFinish.m** automatically executes on a worker each time the worker completes evaluation of a task.

Empty versions of these files are provided in the folder: matlabroot/toolbox/distcomp/user You can edit these files to include whatever MATLAB code you want the worker to execute at the indicated times. Alternatively, you can create your own versions of these files and pass them to the job as part of the AttachedFiles property, or include the path names to their locations in the AdditionalPaths property. The worker gives precedence to the versions provided in the AttachedFiles property, then to those pointed to in the AdditionalPaths property. If any of these files is not included in these properties, the worker uses the version of the file in the toolbox/distcomp/user folder of the worker's MATLAB installation.



#### Slow code? Out of memory?

- Know your enemy:
  - Understand the constraints
  - Identify bottlenecks
- Exploit data and task parallelism
- Find the best tradeoff between programming effort and achieving your goals



#### MATLAB@NSC

- Test your code locally on a small problem first
- Use MATLAB profiler to optimize code and spot parallelizable regions
- Avoid running interactively to the backend, use Batch instead
- Use MATLAB on the desktop as a launcher through the Batch-command





## Speeding up MATLAB Flow-chart











### **Interactively Run a Loop in Parallel**

Create a sine waveform and plot it

Serial version

for i = 1:1024
 A(i) = sin(i\*2\*pi/1024);
end
plot(A)

Parallel version

```
parfor i = 1:1024
    A(i) = sin(i*2*pi/1024);
end
plot(A)
```



\*





#### Parfor variables

- Loop Variable: Loop index
- Sliced Variables: Arrays whose segments are operated on by different iterations of the loop
- Broadcast Variables: Variables defined before the loop whose value is required inside the loop, but never assigned inside the loop
- Reduction Variables: Variables that accumulate a value across iterations of the loop, regardless of iteration order
- Temporary Variables: Variables created inside the loop, and not accessed outside the loop



- The body of a parfor-loop cannot contain another parfor-loop.
- A parfor-loop can call a function that contains another parfor-loop.
- A worker cannot open a parallel pool. Thus, a worker cannot run an inner nested parfor-loop in parallel.
- Only one level of nested parfor-loops can run in parallel.
- If the outer loop runs in parallel on a parallel pool, the inner loop runs serially on each worker.
- If the outer loop runs serially in the client, the function that contains the inner loop can run the inner loop in parallel on workers in a pool.
- The body of a parfor-loop can contain for-loops.
- You can use the inner loop variable for indexing the sliced array, but only in plain form, not part of an expression.



parfor x = 1:jM1 = magic(10000);for y = 1:kM2=zeros(size(M1)); M2(x,y) = x\*10 + y + M1(x,y)/10000;end tic: end [i,k]=size(M1); t(2)=toc;0.3993 sec for x = 1:jfor y = 1:kfor x = 1:i $M2(x,y) = x^{*}10 + y + M1(x,y)/10000;$ parfor y = 1:kend M2(x,y) = x\*10 + y + M1(x,y)/10000;end end end t(1)=toc; t(3)=toc; 3.6440 sec



#### Invalid

```
A = zeros(100, 200);
parfor i = 1:size(A, 1)
    for j = 1:size(A, 2)
        A(i, j) = plus(i, j);
        end
end
```

#### Valid

```
A = zeros(100, 200);
n = size(A, 2);
parfor i = 1:size(A,1)
    for j = 1:n
        A(i, j) = plus(i, j);
        end
end
```

For proper variable classification, the range of a for-loop nested in a parfor must be defined by constant numbers or variables. In the example, the code on the left does not work because the for-loop upper limit is defined by a function call. The code on the right works around this by defining a broadcast or constant variable outside the parfor first.



#### Invalid

#### Valid

```
A = zeros(4, 11);
parfor i = 1:4
   for j = 1:10
        A(i, j + 1) = i + j;
   end
end
```

```
A = zeros(4, 11);
parfor i = 1:4
   for j = 2:11
        A(i, j) = i + j - 1;
        end
end
```

The index variable for the nested for-loop must never be explicitly assigned other than in its for-statement. When using the nested for-loop variable for indexing the sliced array, you must use the variable in plain form, not as part of an expression. In the example, the code on the left does not work, but the code on the right does:



#### Invalid

```
A = zeros(4, 10);
parfor i = 1:4
    for j = 1:10
        A(i, j) = i + j;
    end
        disp(A(i, 1))
end
```

#### Valid

```
A = zeros(4, 10);
parfor i = 1:4
    v = zeros(1, 10);
    for j = 1:10
        v(j) = i + j;
    end
        disp(v(1))
        A(i, :) = v;
end
```

If you use a nested for-loop to index into a sliced array, you cannot use that array elsewhere in the parfor-loop. In the example, the code on the left does not work because A is sliced and indexed inside the nested for-loop; the code on the right works because v is assigned to A outside the nested loop:



#### Invalid

#### Valid

```
A = zeros(4, 10);
A = zeros(4, 10);
                           parfor i = 1:4
parfor i = 1:4
                              for j = 1:10
   for j = 1:5
                                  if j < 6
      A(i, j) = i + j;
                                     A(i, j) = i + j;
   end
                                  else
   for k = 6:10
                                     A(i, j) = pi;
      A(i, k) = pi;
                                  end
   end
                              end
end
                           end
```

Inside a parfor, if you use multiple for-loops (not nested inside each other) to index into a single sliced array, they must loop over the same range of values. Furthermore, a sliced output variable can be used in only one nested for-loop. In the example, the code on the left does not work because j and k loop over different values; the code on the right works to index different portions of the sliced array A:



#### Example: parameter sweep

- Offload parameter sweep to local workers
- Get peak value results when processing is complete
- Plot results in local MATLAB






#### Parameter sweep speedup





#### feval - parfeval

feval – evaluate function

>>y=3

 $x^2 = 2;$ y = feval(fun,x1,x2)

>>y=3.1400

parfeval - Execute function asynchronously on parallel pool worker

f = parfeval(p,@magic,1,10); value = fetchOutputs(f);



#### Parfeval example

```
n = 1000000;
job = cell(1,6);
for idx = 1:6
       jobs(idx) = parfeval(pool, @test, 1, n, idx);
end
% wait for outputs as they finish
output = cell(1, 6);
for idx = 1:6
       [completedIdx, value] = fetchNext(jobs);
      output{completedIdx} = value;
end
delete(pool);
```









#### Overview

- spmd (Single Program Multiple Data)
- labindex and numlabs
- Exchanging data between workers explicitly
- Data transfer to the client using composite arrays





- Similar to parfor, spmd requires a parpool in order for code to run on workers
- If a parpool doesn't exist, one will start if that is the default behavior



#### spmd

- Code inside spmd blocks run on all workers
- Unlike parfor, variables maintain state between calls to spmd as well as in parfor
- Can be used for loading data to be used in parfor loops

```
spmd
    % myfile.mat needs to be available on workers
    data = load('myfile.mat');
end
parfor I = 1:N
    % loop using data
end
```



#### labindex and numlabs

- Helps control what is executed on a worker
- Inside a spmd block
  - labindex returns the rank of the worker
  - numlabs returns the total number of workers in the pool





# Create a Variant Array on Each of the Workers

```
>> magic_squares
spmd
% Build magic squares in parallel
    m = magic(labindex + 2);
end
for ii=1:length(m)
% Plot each magic square
    M = m{ii};
    figure, imagesc(M);
end
```



```
>> approx_pi
```





#### Composite Arrays

- Composite: client-side data-type for viewing data on the workers
- Outside of spmd, index with () or { } to get the data of one of the workers to the client





```
>> spmd, x = labindex/numlabs, end
Lab 1:
 x =
      0.5000
Lab 2:
 x =
       1
>> x
x =
   Lab 1: class = double, size = [1 1]
   Lab 2: class = double, size = [1 1]
>> y = x\{1\}
y =
    0.5000
\rightarrow whos x y
                            Bytes Class Attributes
 Name
            Size
            1x2
                               697
                                   Composite
  х
            1x1
                                 8
                                    double
  У
```



### Types of Composite Arrays (nondistributed arrays)

• Replicated

spmd, x = numlabs, end

• Variant

spmd, x = labindex, end

• Private

spmd, if labindex==1, x = rand, end, end



#### Limitations

• The body of an spmd statement must be transparent



spmd
 data = load(['X' num2str(labindex)]);
 y = data.x;
end



### **Distributed Arrays**



#### Overview

- Distributed Arrays
- Constructing Distributed Arrays
- distributed and codistributed
- Working with Distributed Arrays





- Similar to spmd, distributed arrays require a parpool in order for code to run on workers
- If a parpool doesn't exist, one will start if that is the default behavior



### **Distributed Arrays**

• One variable, split over multiple workers



- However, the MATLAB client sees the variable as one
- Mainly of interest with a cluster, combining the memory of multiple machines
- If the function has been overloaded for distributed arrays, there should be minimal changes to the code



### Creating Distributed Arrays (1)

- Matrix creation functions have been overloaded for distributed arrays
  - zeros(...,'distributed');
  - randn(..., 'distributed');





• If a variable has the same value on all of the workers, use distributed directly



### Creating Distributed Arrays (2)

- Use case: creating a large matrix from multiple files or one large file would not fit into the memory of one computer
- Create data on each worker
- Combined into a distributed array using codistributed.build and codistributed1d



• Specify the size of the distributed array and optionally the partitioning



### Working with Distributed Arrays

- A collection of MATLAB functions are overloaded for distributed arrays
- Overloaded functions can be called similar to other data types (e.g. numeric)

>> methods distributed

abs acos acos acos acot acot acot acot acsc acsc all and angle any ...

• Call gather to convert back to a numeric array



#### Using Distributed Arrays on Workers

#### >> distrib\_example

```
W = ones(8,'distributed'); % Distribute to the workers
spmd
T = W*2; % Calculation performed on workers, in parallel.
% T and W are both codistributed arrays here.
end
T % View results in client.
whos % T and W are both distributed arrays here.
```



#### distributed and codistributed

- The same distributed array will have a data type of:
  - distributed: on the client
  - codistributed: on the workers (within a spmd block)





#### Using Codistributed Arrays on Workers

```
>> codistrib_example
```

```
p = parpool(2);
spmd
% Define 1-D distribution along the 3rd dimension
% 4 parts on worker 1, and 12 parts on worker 2
codist = codistributor1d(3,[4,12]);
Z = zeros(3,3,16,codist);
Z = Z + labindex;
end
Z % View results in client (distributed array here)
```





#### **GPU-computing**



#### What is needed?

- Matlab
- PCT
- GPU



#### Suitable problems

- Massively parallel tasks
- Computationally intensive tasks
- Tasks that have limited kernel size



### Options

- Built-in functions
- Functions on array data
- Directly invoke CUDA-code



#### Control vs Effort





#### **Built-in functions**

- Accelerate standard (highly parallel) functions

   More than 200 MATLAB functions are already
   supported
- Out of the box:

111	010
Matrix multiplications	Cho
Solvers	
Convolutions	

Min/max SVD Cholesky and LU factorization

- No additional effort for programming the GPU
- No accuracy for speed trade-off
  - Double floating-point precision computations





maxIterations = 500;

gridSize=1000;

xlim = [-0.748766713922161, -0.748766707771757];

ylim = [ 0.123640844894862, 0.123640851045266];

#### t = tic();

```
x = linspace( xlim(1), xlim(2), gridSize );
y = linspace( ylim(1), ylim(2), gridSize );
[xGrid,yGrid] = meshgrid( x, y );
z0 = xGrid + li*yGrid;
```

count = ones( size(z0) );

% Calculate

```
z = z0;
```

for n = 0:maxIterations

 $z = z \cdot z + z0;$ 

inside = abs(z) <=2;

count = count + inside;

 $\operatorname{end}$ 



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% show



```
t = tic();
x = gpuArray.linspace( xlim(1), xlim(2), gridSize );
y = gpuArray.linspace( ylim(1), ylim(2), gridSize );
[xGrid,yGrid] = meshgrid( x, y );
z0 = complex( xGrid, yGrid );
count = ones( size(z0), 'gpuArray' );
```

```
% Calculate
```

```
z = z0;
```

```
for n = 0:maxIterations
```

 $z = z \cdot z + z0;$ 

```
inside = abs( z )<=2;</pre>
```

count = count + inside;

#### end

```
count = log( count );
```

#### % Show

count = gather( count ); % Fetch the data back from the GPU

naiveGPUTime = toc( t );



## Example cont'd

t = tic();

x = gpuArray.linspace( xlim(1), xlim(2), gridSize ); y = gpuArray.linspace( ylim(1), ylim(2), gridSize ); [xGrid,yGrid] = meshgrid( x, y );

% Calculate

```
count = arrayfun( @pctdemo_processMandelbrotElement, ...
```

xGrid, yGrid, maxIterations );

% Show

count = gather( count ); % Fetch the data back from the GPU
gpuArrayfunTime = toc( t );

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#### Example cont'd

% Load the kernel

cudaFilename = 'pctdemo\_processMandelbrotElement.cu';

ptxFilename = ['pctdemo\_processMandelbrotElement.',parallel.gpu.ptxext];

kernel = parallel.gpu.CUDAKernel( ptxFilename, cudaFilename );

% Setup

```
t = tic();
```

```
x = gpuArray.linspace( xlim(1), xlim(2), gridSize );
```

```
y = gpuArray.linspace( ylim(1), ylim(2), gridSize );
```

```
[xGrid,yGrid] = meshgrid( x, y );
```

% Make sure we have sufficient blocks to cover all of the locations numElements = numel( xGrid ); kernel.ThreadBlockSize = [kernel.MaxThreadsPerBlock,1,1]; kernel.GridSize = [ceil(numElements/kernel.MaxThreadsPerBlock),1];

% Call the kernel

```
count = zeros( size(xGrid), 'gpuArray' );
```

count = feval( kernel, count, xGrid, yGrid, maxIterations, numElements );

```
// Generated by NVIDIA NVVM Compiler
 11
 // Compiler Build ID: CL-19856038
 // Cuda compilation tools, release 7.5, V7.5.17
 // Based on LLVM 3.4svn
  .version 4.3
  .target sm 20
  .address size 64
                    // .globl
                                       Z12doIterationsddj
 device
unsigned int doIterations( double const realPart0,
                             double const imagPart0,
                             unsigned int const maxIters ) {
   // Initialize: z = z0
   double realPart = realPart0;
   double imagPart = imagPart0:
   VCC d inptxtC
   while ( ( count <= maxIters )
          && ((realPart*realPart + imagPart*imagPart) <= 4.0) ) {</pre>
                    0%pl bra
                                       BB0 3;
                    add.s32
                                       %r6, %r6, 1;
                    sub.f64
                                       %fd10, %fd4, %fd3;
                    add, f64
                                       %fd5, %fd10, %fd7;
                    add.f64
                                       %fd11, %fd2, %fd2;
                    fma.rn.f64
                                       %fd6, %fd11, %fd1, %fd8;
                    setp.le.u32
                                       %p2, %r6, %r4;
```

:	st.param.b32 ret;	[func_retval0+0],	ST GAR SI

%fd12, %fd6:

%fd13, %fd5;

BB0 1:

mov.f64

mov.f64

@%p2 bra

BB0 3



#### Example cont'd

ans: 'finished'

count: [1000x1000 double] cpuTime: 15.9700 gpuArrayfunTime: 0.7010 gridSize: 1000 inside: [1x1 gpuArray] maxIterations: 500 n: 500 naiveGPUTime: 5.5109 t: 1443545040634310 x: [1x1 gpuArray] xGrid: [1x1 gpuArray] xlim: [-0.7488 -0.7488] y: [1x1 gpuArray] yGrid: [1x1 gpuArray] ylim: [0.1236 0.1236] z: [1x1 gpuArray] z0: [1x1 gpuArray]

#### Laptop 6.24s


## Ma Simple example

k = parallel.gpu.CUDAKerne('test.ptx','test.cu');

result = feval(k,2,3)



## Multiple GPUs

parpool(2)
spmd
gd=gpuDevice;
idx=gd.Index;
disp(['Using GPU ',num2str(idx)]);
end
parfor ix = 1:10
gd=gpuDevice;
d(ix)=gd.Index;
end







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