

Workshop: Parallel Computing with MATLAB

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Outline

- Introduction to Parallel Computing Tools
- Using Parallel Computing Toolbox
 - Task Parallel Applications
 - Data Parallel Applications



Parallel Computing with MATLAB





Parallel Computing with MATLAB





Solving Big Technical Problems



Large data set

Reduce size of problem



Load *data* onto multiple machines that work together in *parallel*



Parallel Computing Toolbox API

Task-parallel Applications

- Using the parfor constructs
- Using jobs and tasks

Data-parallel Applications

- Using distributed arrays
- Using the spmd construct



Task-parallel Applications

- Converting for to parfor
- Configurations
- Scheduling parfor
- Creating jobs and tasks
- When to Use parfor vs. jobs and tasks
- Resolving parfor Issues
- Resolving jobs and tasks Issues



Toolboxes with Built-in Support

- Optimization Toolbox
- Global Optimization Toolbox
- Statistics Toolbox
- Simulink Design Optimization
- Bioinformatics Toolbox
- Communications Toolbox



Contain functions that directly leverage functions from the Parallel Computing Toolbox



Opening and Closing a matlabpool...





Open and close a matlabpool with two labs



Determining the Size of the Pool...

A Command Window	_ <u>_</u> _×
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>> matlabpool size	
ans =	
2	
fx >>	
	OVR



One Pool at a Time



Even if you have not exceeded the number of labs, you can only open one matlabpool at a time



Add Shortcut for Starting the matlabpool

🥠 Short	cut Editor	- 0 ×
Label:	Open local Pool	
Callback:	<pre>if matlabpool('size')==0 matlabpool open local 2 end</pre>	
Category:	Toolbar Shortcuts	•
Icon:	MATLAB icon	•
Saves sl Shortcul	hortcut to Start button. Selecting "Toolbar Shortcuts" category also s ts toolbar. Save Cancel <u>H</u> elp	aves to



Add Shortcut for Stopping the matlabpool

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Category:	Toolbar Sh	ortcuts			•
Icon:		B icon			•
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Example: Parameter Sweep of ODEs

Solve a 2nd order ODE

$$\vec{m} \ddot{x} + \underbrace{b}_{1,2,\dots} \dot{x} + \underbrace{k}_{1,2,\dots} x = 0$$

- Simulate with different values for *b* and *k*
- Records and plots peak values





\task_parallel\paramSweepScript.m



The Mechanics of parfor Loops



Pool of MATLAB Workers



Converting for to parfor

Requirements for parfor loops

- Task independent
- Order independent
- Constraints on the loop body
 - Cannot "introduce" variables (e.g. eval, load, global, etc.)
 - Cannot contain break or return statements
 - Cannot contain another parfor loop



Advice for Converting for to parfor

- Use M-Lint to diagnose parfor issues
- If your for loop cannot be converted to a parfor, consider wrapping a subset of the body to a function
- Read the section in the documentation on classification of variables
- http://blogs.mathworks.com/loren/2009/10/02/usingparfor-loops-getting-up-and-running/



Resolving parfor **Issues**

 Let's look at a common parfor issues and how to go resolving them



Unclassified Variables



The variable A cannot be properly classified

task_parallel\valid_indexing_error.m



parfor Variable Classification

 All variables referenced at the top level of the parfor must be resolved and <u>classified</u>

Classification	Description
Loop	Serves as a loop index for arrays
Sliced	An array whose segments are operated on by different iterations of the loop
Broadcast	A variable defined before the loop whose value is used inside the loop, but never assigned inside the loop
Reduction	Accumulates a value across iterations of the loop, regardless of iteration order
Temporary	Variable created inside the loop, but unlike sliced or reduction variables, not available outside the loop



Variable Classification Example

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	1		a =	0;								
	2		c =	pi;								
	3		z =	0;								
	4		r =	ran	nd(1	,10);	:					
	5	E	part	Eor	idx	= 1	:10	←───	Loop variat	ole		
Temporary variable	6		<u>,</u>	a =	idx	;						
Reduction variable	-7			z =	z+i	dx;						
Sliced output variable	-8		->1	o(io	ix)	= r(:	idx);	<	Sliced inpu	it variable)	
	9			if :	idx<	=c		< ──	Broadcast	variable		
	10			0	1 =	2*a;						
	11			and								
	12		end									
	13											
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At the end of this loop, what is the value of each variable?

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1		a =	one	es (1	,10);	(
2		e =	0;								
3		f =	5;								
4		g =	0;								
5		h =	10	;							
6	E	par	for	idx	= 1:	10					
7]	=	2*a	;						
8				a(i	dx);						
9			d(id	dx)	= id>	;					
10			e =	e+i	dx;						
11			£ =	idx	;						
12			g =	g+2	;						
13		1	h =	20;							
14		end									
15											
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task_parallel\what_is_it_parfor.m

📣 The MathWorks[.]

Results

- a: ones(1:10) (broadcast)
- b: undefined (temp)
- c: undefined (temp)
- d: 1:10 (sliced)
- e: 55 (reduction)
- f: 5 (**temp**)
- g: 20 (reduction)
- h: 10 (**temp**)
- idx: undefined (loop)

-10	Intitle	d*									
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1		a =	one	es (1	,10);						1
2		e =	0;								
3		f =	5;								
4		g =	0;								
5		h =	10	;							
б	E	par	for	idx	= 1:	:10					
7		3	= 0	2*a	;						
8			c =	a(i	dx);						
9			1(10	(xh	= idx	(;					
10			e =	e+i	dx;						
11		10	f =	idx	;						
12		19	g =	g+2	;						
13		. 1	h =	20;							
14		end									
15											
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parfor issue: Nested for loops



Within the list of indices for a sliced variable, one of these indices is of the form i, i+k, i-k, k+i, or k-i, where i is the loop variable and k is a constant or a simple (non-indexed) variable; and every other index is a constant, a simple variable, colon, or end.



parfor issue: Solution 1

1	ntitle	d*											×
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1		A =	zei	cos (10);								
2													
3	E	part	for	i =	1:10)							
4		3	o =	zer	os(1,	10);							
5	E		for	j =	1:10)							
6			1	(j)	= i+	-j;							
7			end										
8			A(i,	;;)	= b;								
9		end											
10													
			ſ	script				Ln	10	Col	1	OVR	1

Create a temporary variable, b to store the row vector. Use the looping index, i, to index the columns and the colon to assign the row vector to the temporary variable between the for loops.

task_parallel\valid_indexing_fix1.m



parfor issue: Solution 2

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1 % A = zeros(10);
2 - A = cell(10, 1);
3
4
$5 - \Box$ for j = 1:10
$6 - A{i}(j) = i+j;$
7 - end
8 - end
9
10 - A = cell2mat(A);

Use cell arrays. The restrictions on indexing only apply to the top-level indexing (i.e. indexing into the cell array). Indexing into contents of the cell arrays is allowed.

task_parallel\valid_indexing_fix2.m



Using parfor with Simulink

- Can use parfor with sim.
- Must make sure that the Simulink workspace contains the variables you want to use.
- Within main parfor body: Use `base' workspace
- Use assignin to place variables in base workspace.
- Note: the base workspace when using parfor is different than the base workspace when running serially.



Parallel Computing Tools Address...





Data-parallel Applications

- Using distributed arrays
- Using spmd
- Using mpi based functionality



Client-side Distributed Arrays



Remotely Manipulate Array from Desktop

Distributed Array Lives on the Cluster



Client-side Distributed Arrays and SPMD

Client-side distributed arrays

- Class distributed
- Can be created and manipulated directly from the client.
- Simpler access to memory on labs
- Client-side visualization capabilities
- spmd
 - Block of code executed on workers
 - Worker specific commands
 - Explicit communication between workers
 - Mixture of parallel and serial code



spmd blocks (Data Parallel)

spmd % single program across workers end

- Mix data-parallel and serial code in the same function
- Run on a pool of MATLAB resources
- Single Program runs simultaneously across workers
 - Distributed arrays, message-passing
- <u>Multiple Data spread across multiple workers</u>
 - Data stays on workers

data_parallel\spmd_example.m



The Mechanics of spmd Blocks



Pool of MATLAB Workers



Composite Arrays

- Created from client
- Stored on workers
- Syntax similar to cell arrays





Composite Array in Memory

>> matlabpool open 4 >> x = Composite(4)>> $x\{1\} = 2$ >> $x\{2\} = [2, 3, 5]$ >> $x{3} = 0 \sin$ $x \rightarrow$ >> $x{4} = tsobject()$





spmd

- single program, multiple data
- Unlike variables used in multiple parfor loops, distributed arrays used in multiple spmd blocks retain state
- Use M-Lint to diagnose spmd issues



Noisy Image – too large for a desktop





Distribute Data





Distribute Data















Pass Overlap Data















Pass Overlap Data





Pass Overlap Data















Apply Median Filter















Combine as Distributed Data









Combine as Distributed Data





MPI-Based Functions in Parallel Computing Toolbox

Use when a high degree of control over parallel algorithm is required

- High-level abstractions of MPI functions
 - labSendReceive, labBroadcast, and others
 - Send, receive, and broadcast any data type in MATLAB
- Automatic bookkeeping
 - Setup: communication, ranks, etc.
 - Error detection: deadlocks and miscommunications
- Pluggable
 - Use any MPI implementation that is *binary*-compatible with MPICH2

Summary for Interactive Functionality

Client-side Distributed Arrays

- MATLAB array type across cluster
- Accessible from client
- SPMD ... END

'he MathWorks™

- Flow control from serial to parallel
- Fine Grained
- More control over distributed arrays
- Composite Arrays
 - Generic data container across cluster
 - Accessible from client





Migrating from Interactive to Scheduled





Interactive to Scheduled

Interactive

- Great for prototyping
- Immediate access to MATLAB workers
- Scheduled
 - Offloads work to other MATLAB workers (local or on a cluster)
 - Access to more computing resources for improved performance
 - Frees up local MATLAB session



Using Configurations

Managing configurations

- Typically created by Sys Admins
- Label configurations based on the version of MATLAB
 - E.g. linux_r2009a
- Import configurations generated by the Sys Admin
 - Don't modify them with two exceptions
 - Setting the CaptureCommandWindowOutput to true for debugging
 - Set the ClusterSize for the local scheduler to the number of cores



Creating and Submitting Jobs





Rather than using a shell script to submit a job to a cluster, we'll write our *jobscript* in MATLAB.

task_parallel\basic_jobscript.m



Example: Scheduling the ODE Sweep

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Ç <mark>e</mark>	$-1.0 + \div 1.1 \times \% \% 0$
ş	<pre>%% Get handle to the job scheduler</pre>
5	<pre>sched = findResource();</pre>
4	%% Create a matlabpool job
ę	<pre>% Split among pool of 2 labs, 1 lab acts as serial MATLAB does (total = 3)</pre>
r	nlabs = 3;
	job = createMatlabPoolJob(sched,
	'FileDependencies', {'paramSweep.m'},
	'MinimumNumberOfWorkers', nlabs,
	'MaximumNumberOfWorkers', nlabs);
2	<pre>set(job,'Tag','MyODEJob') % Can use Tag to label jobs, not necessary</pre>
4	%% Create a single parfor task
t	<pre>task = createTask(job,@paramSweep,1,{});</pre>
ş	%% Submit the job and wait
\$	submit(job)

task_parallel\jobscript_ode.m



Example: Retrieving Results



task_parallel\ode_return.m



Considerations When Using parfor

- parfor automatically quits on error
- parfor doesn't provide intermediate results



Creating Jobs and Tasks

 Rather than submitting a single task containing a parfor, the jobscript can be used to create an array of tasks, each calling a unit of work



Example: Using Multiple Tasks

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$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	
1 %% Submitting Jobs and Tasks	
2	
3 %% Get handle to the job scheduler	
4 - sched = findResource();	
5	
6 %% Create a simple distributed job	
<pre>7 - job = createJob(sched, 'FileDependencies', {'myfcn.m'});</pre>	
8	
9 %% Create the tasks	
10 - 🕞 for tidx = 1:10	
<pre>11 - tasks(tidx) = createTask(job,@myfcn, 1, {tidx}); %#ok<sagrow></sagrow></pre>	
12 - end	
13	
14 - submit(job)	
15	

task_parallel\jobscript_tasks.m



Example: Retrieving Task Results

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[□] *= □] - 1.0 + ÷ 1.1 × ½ ½ 0 .	
1 %% Retrieving Output from Jobs and Tasks	
2	
3 %% Check to make sure job is finished	
4	
5 – job.State	
6	
7 %% Once finished, get output (method 1, all at once)	
8	
<pre>9 - output = getAllOutputArguments(job);</pre>	
10 - celldisp(output)	
11	
12 %% Once finished, get output (method 2, output of specific task)	
13	
14 - job.task(1).State % how to check state of particular task	
<pre>15 - output = job.task(1).OutputArguments; % output from task 1</pre>	
16 - celldisp(output)	
17	
18 %% Destroy job when finished	
19	
20 - destroy(job)	
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task_parallel\tasks_return.m



Resolving Jobs & Tasks Issues

- Code running on your client machine ought to be able to resolve functions on your path
- When submitting jobs to a cluster, those files need to either be submitted as part of the job (FileDependencies) or the folder needs to be accessible (PathDependencies)
- There is overhead when adding too many files to the job; but setting path dependencies requires the Worker to be able to reach the path



parfor or jobs and tasks

parfor

- Seamless integration to user's code
- Several for loops throughout the code to convert
- Automatic load balancing

Jobs and tasks

- All tasks run
- Query results after each task is finished

Try parfor first. If it doesn't apply to your application, create jobs and tasks.



Example: Scheduling Estimating π

What is the probability that a randomly dropped needle will cross a grid line?

a

(Buffon-Laplace Method) Simulate random needles dropping, calculate P, and get an estimate for π .

$$P(l,a,b) = \frac{2l(a+b) - l^2}{\pi ab} = \frac{\text{crossing needles}}{\text{total needles}}$$

data parallel\jobscript Pi.m



Summary for Scheduled Functionality

	uses matlabpool	function	script	pure task parallel	pure data parallel	parallel and serial
batch	\checkmark		✓			✓
matlabpool job	\checkmark	\checkmark				✓
jobs and tasks		✓		~		
parallel job		\checkmark			\checkmark	





- Profile your code to search for bottlenecks
- Make use of M-Lint when coding parfor and spmd
- Beware of writing to files
- Avoid the use of global variables
- Run locally before moving to cluster