Parallel Computing with Matlab
UVACSE Short Course

Ed Hall[1]

[1]University of Virginia Alliance for Computational Science and Engineering
uvacse@virginia.edu

October 5, 2011

Outline

Outline

Starting and Configuring NX Client

Starting NX Client

- On classroom computer, search for and start NX client
- On personal computer, download and install NX client
  http://www.nomachine.com/download.php

Configuring NX Client

- Session: The name you choose to refer to the host
- Host: This must be the full qualified name, e.g. fir.itc.virginia.edu
- Move the slider to WAN
- Change the desktop from KDE to Gnome.
  http://www.uvacse.virginia.edu/the-nx-client/

Starting and Configuring NX Client

Once logged into `fir.itc.virginia.edu` through NX

- Open a terminal from Applications/Accessories/Terminal menu
  - Select and right-click on Terminal to add to launcher
- Create a `Matlab` directory with `mkdir` command
- Start web browser from icon at top of desktop

Outline

Download Short Course Examples

Download the short-course materials from
http://www.uvacse.virginia.edu/software/Matlab-at-uva/

Follow the links,
→High Performance Computing
→Parallel Computing Toolbox
→Parallel Computing Short Course
and download 3 files to `Matlab` directory you create with `mkdir` command

- ClassExamples.zip
- ClassSlides.pdf
- ParallelMatlabCluster.pdf

Outline

Solving Big Technical Problems

- Computationally intensive, long-running codes
  - Run tasks in parallel on many processors
  - Task parallel
- Large Data sets
  - Load data across multiple machines that work in parallel
  - Data parallel

Solving Big Technical Problems

- Parallel Computing Toolbox solves computationally and data-intensive problems using Matlab
- Parallel processing language constructs let you implement task- and data-parallel algorithms in Matlab at a high level
  - parallel for-loops and code blocks
  - distributed arrays, parallel numerical algorithms
  - message-passing functions
- Perform parallel computations on multicore computers and computer clusters

Outline

Parallel Computing Toolbox Features

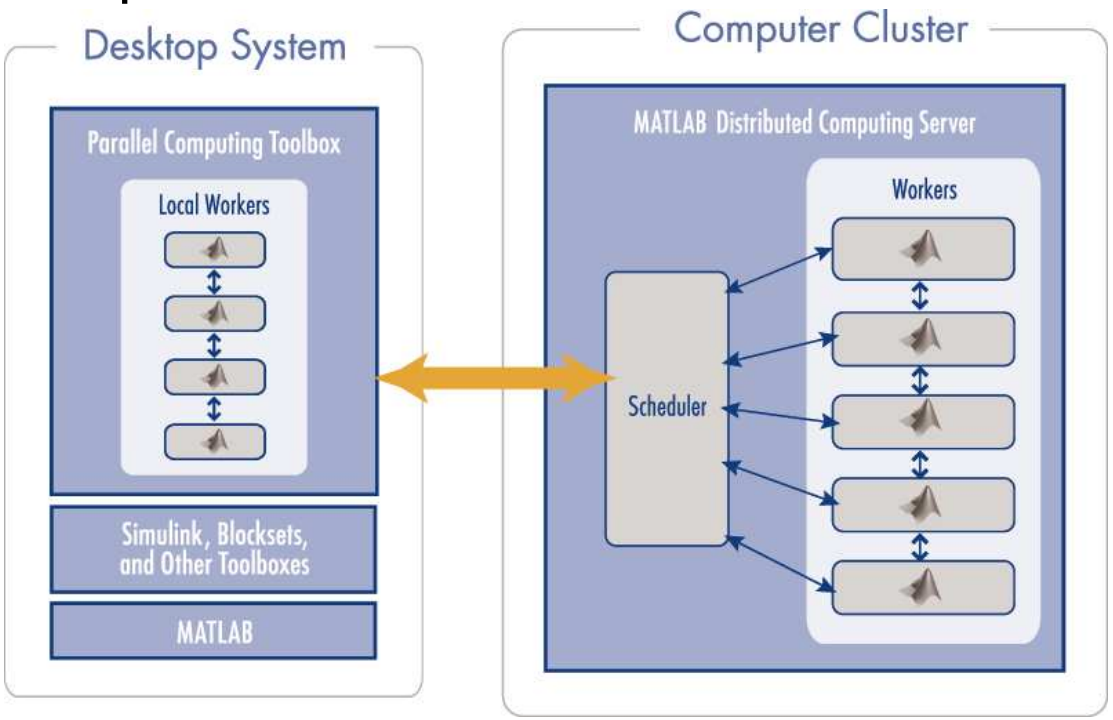
- Support for **data-parallel** and **task-parallel** application development
- Ability to annotate code segments
  - **`parfor`** (parallel for-loops) for task-parallel algorithms
  - **`spmd`** (single program multiple data) for data-parallel algorithms
- **Interactive** and **batch** execution modes for efficient computational workflow.
- Run eight workers locally on a multicore desktop
- Integration with Matlab Distributed Computing Server for **cluster-based applications** that use any scheduler or **any number of workers**

Programming Parallel Applications in Matlab

- Several **high-level programming constructs** that let you convert your serial Matlab code to run in parallel on several workers
- Simplify parallel code development by abstracting away the complexity of managing coordination and distribution of computations and data between a Matlab client and workers
- The parallel programming constructs function even in the absence of workers, letting you maintain a single version of your code for both serial and parallel execution

Matlab Parallel Workflow

The toolbox enables application prototyping on the desktop with up to eight local workers (left), and with Matlab Distributed Computing Server (right), applications can be scaled to multiple computers on a cluster.



UseParallel for Optimization Algorithms

The Optimization Toolbox solvers **`fmincon`**, **`fgoalattain`**, and **`fminimax`** can automatically distribute the numerical estimation of gradients of objective functions and nonlinear constraint functions to multiple processors.

- Parallel computing is enabled with **`matlabpool`**, a Parallel Computing Toolbox function
- The option **`UseParallel`** is set to **`'Always'`**. The default value of this option is 'Never'.

UseParallel for Optimization Algorithms

Optimization Toolbox

- **`fmincon`**
- **`fminimax`**
- **`fgoalattain`**

Genetic Algorithm and Direct Search Toolbox

- **`ga`**
- **`gamultiobj`**
- **`patternsearch`**

UseParallel for Optimization Algorithms

- The built-in parallel support in Optimization Toolbox is **beneficial for problems that have objective/constraint functions with execution times greater than network overhead** associated with distributing computations across multiple workers

- However, **parallelizing the objective/constraint function itself can be a better approach** if it is the most expensive step in the optimization problem and can be accelerated by parallelizing the objective function

Documentation:
Improving Optimization Performance with Parallel Computing

Example Code: Parallel Optimization with `fmincon`

```
% Serial Use of fmincon
startPoint = [1 -2 0 5];
options = optimset('Display','iter','Algorithm','active-set');
startTime = tic;
fmincon(@expensive_objfun,startPoint,[],[],[],[],[],[],...
    @expensive_confun,options);
time_fmincon_sequential = toc(startTime);
fprintf('Serial FMINCON optimization takes %g seconds.\n', ...
    time_fmincon_sequential);

% Parallel Use of fmincon
matlabpool open 2 % open matlab pool of two workers
% Set fmincon options
options = optimset(options,'UseParallel','always');
startTime = tic;
fmincon(@expensive_objfun,startPoint,[],[],[],[],[],[],...
    @expensive_confun,options);
time_fmincon_parallel = toc(startTime);
fprintf('Parallel FMINCON optimization takes %g seconds.\n',...
    time_fmincon_parallel);
matlabpool close % close matlab pool
```

Minimizing an Expensive Optimization Problem Using Parallel Compu

Task-parallelism using `parfor`

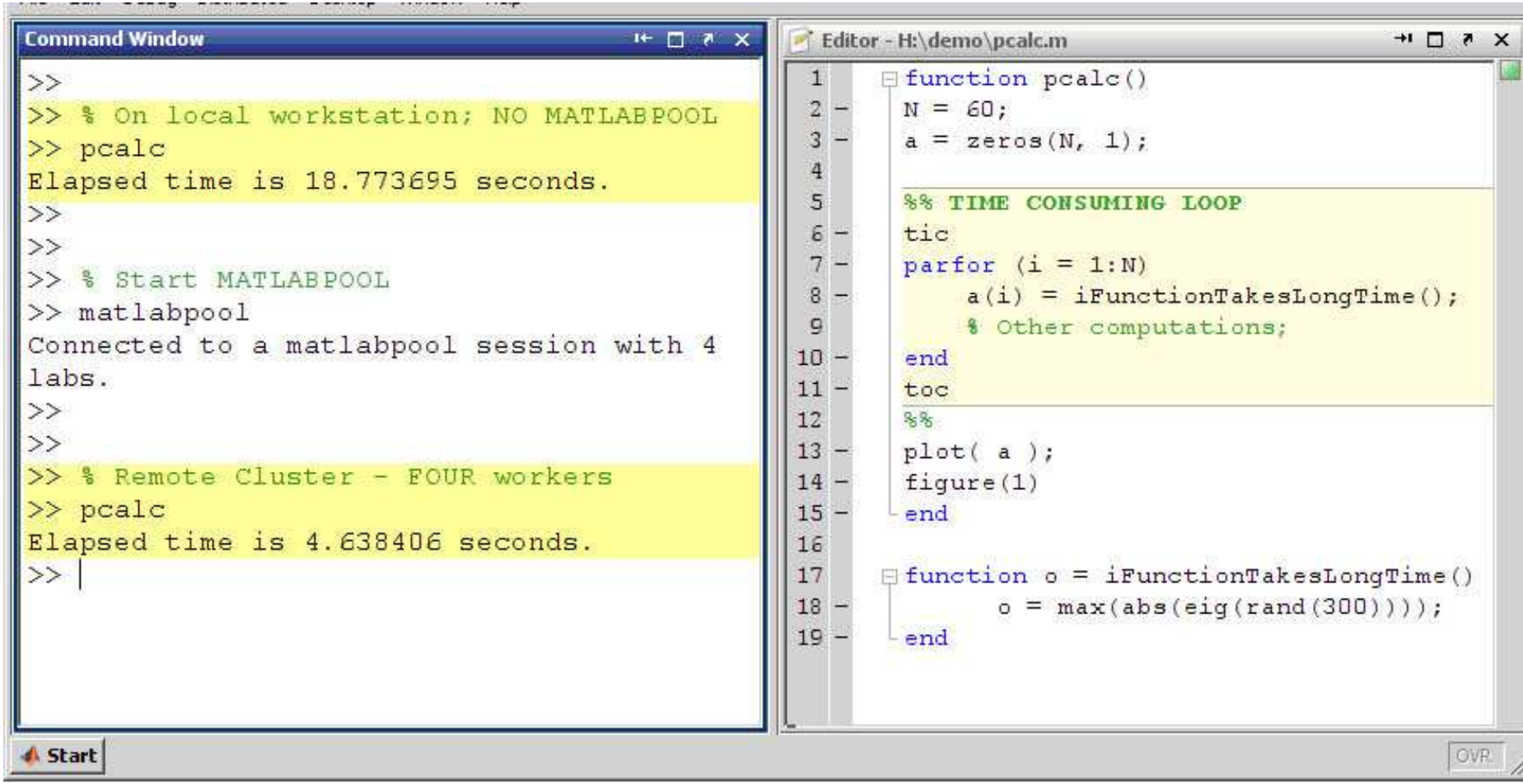
Parallel `for`-Loops - `parfor`

- Code Annotation

```
parfor i = 1 : n
   % do something with i
end
```

- Mix task-parallel and serial code in the same function
- Run loops on a pool of Matlab resources
- Iterations must be order-independent

Task-parallelism using `parfor`



Task-parallelism using `parfor`

- Parallel for-loops (`parfor`) automatically distribute a set of independent tasks over a set of workers.
- Work distribution across worker is dynamic for load balancing.
- The `matlabpool` command sets up the interactive execution environment for parallel constructs such as `parfor` or `spmd` (coming next)
- The running code automatically detects the presence of workers and reverts to serial behavior if none are present.

Task-parallelism using `parfor`

- Using the `createMatlabPoolJob` command allows code using Matlab's parallel constructs to run in batch mode across the compute nodes of a cluster.
- Applications: Monte Carlo simulations, Parameter sweeps

Task-parallelism using `parfor`: Example Code

```
function  pcalc(nloop)
% Example using the parfor construct

N=nloop;
a=zeros(N, 1);

%% TIME CONSUMING LOOP
tic;
parfor i=1:N
    a(i)=iFunctionTakesLongTime();
    % Other computations
end
toc
%%
plot(a);
figure(1)

end

function max_eig=iFunctionTakesLongTime()
% Computation intensive calculation
max_eig=max(abs(eig(rand(300))));
end
```

Setting Up the Matlab Workers

The `matlabpool` Command

- The `matlabpool` command allocates a set of dedicated computational resources
  - reserves a number of Matlab workers and sets up an interactive environment for executing parallel Matlab code
- Parallel Computing Toolbox provides the ability to use up to eight local workers on a multicore or multiprocessor computer using a single toolbox license
- Within this environment, `parfor` and `spmd` constructs can set up data and Matlab code exchange between a Matlab client session and Matlab workers.

spmd for Data-Parallel Processing

- For Matlab algorithms that require large data set processing, Parallel Computing Toolbox provides,
  - distributed arrays, parallel functions
  - the spmd keyword to annotate sections of your code for parallel execution on several workers.
- These parallel constructs handle the inter-worker communication and coordinate parallel computations behind the scenes.

spmd for Data-Parallel Processing

- Using distributed arrays, you can allocate matrices of any data type across all workers participating in the parallel computation.
- Parallel functions let you perform mathematical operations such as indexing, matrix multiplication, decomposition, and transforms directly on distributed arrays.
- The toolbox also provides more than150 parallel functions for distributed arrays, including linear algebra routines based on ScaLAPACK.

spmd for Data-Parallel Processing

Single Program Multiple Data - spmd

- Code Annotation

```
spmd
   % data parallel operation
end
```

- Single program
  - Runs simultaneously across all workers
  - Enables easy writing and debugging
- Multiple Data
  - Data spread across workers
- Runs serially if no workers are available

`spmd` for Data-Parallel Processing

Distributed Arrays

- Distributed arrays are special arrays that store segments of data on Matlab workers that are participating in a parallel computation.
  - can handle larger data sets than you can on a single Matlab session.
- You can construct distributed arrays in several ways:
  - Using constructor functions such as `rand`, `ones`, and `zeros`
  - Concatenating arrays with same name but different data on different labs
  - Distributing a large matrix

spmd for Data-Parallel Processing: Example Code

Solving a Large Linear System

```
>> matlabpool open
Starting matlabpool using the parallel configuration 'local'.
Waiting for parallel job to start...
Connected to a matlabpool session with 4 labs.
>> spmd
    A = rand(N, N, codistributor());
    b = sum(A, 2);
    % solve Ax=b
    [L,U,p] = lu(A, 'vector');
    x = U\(L\(b(p, :)));
    x2 = gather(x);
    % Check error
    errChk = normest(A * x - b);
end
x2=x2{:};
errChk=errChk{:}

errChk =

   1.9194e-11

fx >>
```

spmd for Data-Parallel Processing: Example Code

Solving a Large Linear System

```
>> matlabpool open
Starting matlabpool using the parallel configuration 'local'.
Waiting for parallel job to start...
Connected to a matlabpool session with 4 labs.
>> spmd
    A = rand(N, N, codistributor());
    b = sum(A, 2);
    % solve Ax=b
    [L,U,p] = lu(A, 'vector');
    x = U\(L\(b(p, :)));
    x2 = gather(x);
    % Check error
    errChk = normest(A * x - b);
end
x2=x2{:};
errChk=errChk{:}

errChk =

   1.9194e-11

fx >>
```

spmd for Data-Parallel Processing: Example

Numerical Estimation of Pi Using Message Passing

- Use the fact that

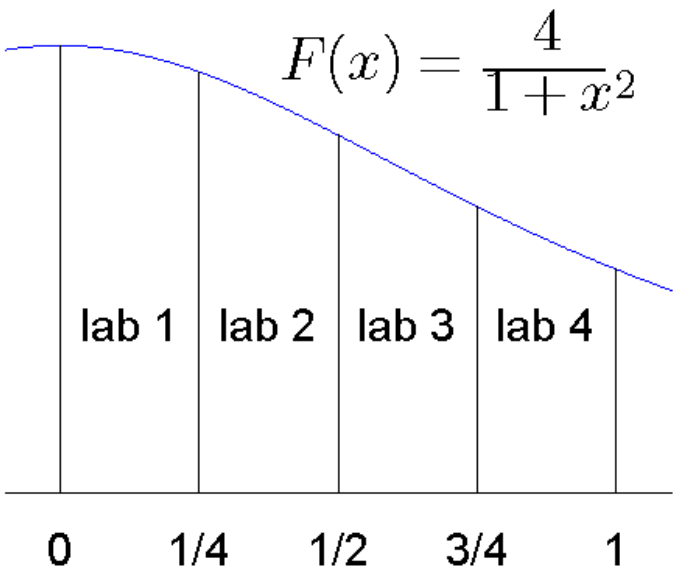
$$\int_0^1 \frac{4}{1+x^2} dx = 4(atan(1) - atan(0)) = \pi \qquad (1)$$

  to approximate pi by approximating the integral on the left

- use the spmd keyword to mark the parallel blocks of code and the Matlab worker pool performs the calculations in parallel

spmd for Data-Parallel Processing: Example

Divide the work between four labs by having each lab calculate the integral of the function over a subinterval of [0, 1]



Define the variables a and b on each lab using the `labindex` so that the intervals [a, b] correspond to the subintervals above.

spmd for Data-Parallel Processing: Example Code

Parallel Esimation of Pi:

```
F = @(x) 4./(1 + x.^2);

spmd
    % Define integration interval
    a = (labindex - 1)/numlabs;
    b = labindex/numlabs;
    [a,b]
    fprintf('Subinterval: [%-4g, %-4g]\n', a, b);

    % Use Matlab quadrature method to approximate integral
    myIntegral = quadl(F, a, b);
    fprintf('Subinterval: [%-4g, %-4g]   Integral: %4g\n', ...
            a, b, myIntegral);

    % We use the gplus function to add myIntegral across all the
    % labs and return the sum on all the labs.
    piApprox = gplus(myIntegral);

end
```

Matlab MPI for Message Passing

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

- High-level abstractions of MPI message-passing routines based on the MPI standard (MPICH2)
  - `labSendReceive`, `labBroadcast`, and others
- Send, receive, and broadcast any data type in Matlab including structures and cell arrays, without any special setup.
- Use any MPI implementation that is binary-compatible with MPICH-2

Message Passing for Data Parallel Algorithms

Message passing functions can be used with `spmd` statements

```
>> matlabpool open 4
Starting matlabpool using the parallel configuration 'local'.
Waiting for parallel job to start...
Connected to a matlabpool session with 4 labs.
>> spmd
    source = 1;
    destination = [2, 4];
    if labindex == source
        % Send data from source lab
        testData.rpm = 1000; % Set up structure
        testData.speed = 35;
        otherData = rand(1000); % A random array

        labSend(testData, destination);
        labSend(otherData, destination);
    elseif any(labindex == destination)
        % Receive on destination labs
        recvdata{1} = labReceive(source);
        recvdata{2} = labReceive(source);
    end
end
>> v=recvdata{2}; % Data received in lab 2
v{1}

ans =

      rpm: 1000
    speed: 35
```

pmode for Interactive Parallel Computing

Parallel Command Window

- The Parallel Command Window provides an extension to the Matlab command window for executing data-parallel Matlab code directly on workers participating in the interactive parallel session
- Commands issued at the pmode prompt are executed immediately on all the labs and results are returned immediately to the client session.
- You can use distributed arrays, associated parallel functions, as well as message-passing functions in this mode.
- This tool facilitates the debugging process, as it allows you to watch the results and the interaction between labs at each step.

pmode for Interactive Parallel Computing

Interactive Prototyping / Development Using Parallel Command Window

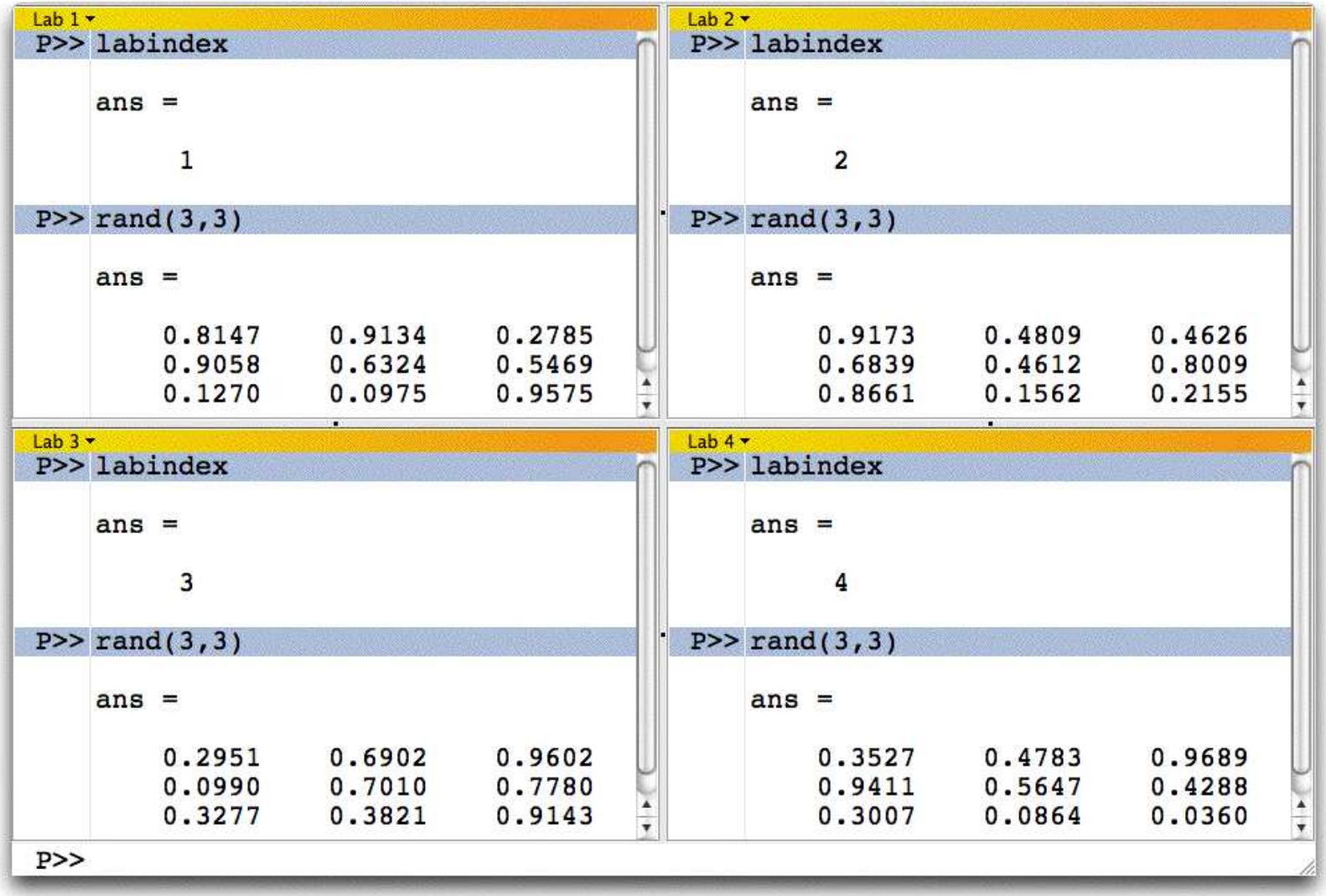
- Parallel Command Window similar to regular command window
- Execute commands and observe behavior on each worker of the cluster
- Can run up to 8 workers on Matlab desktop
- Workers are processes, not tied to cores or processors as such

pmode for Interactive Parallel Computing

Example Code

```
>>pmode start
P>>a=1
P>>labindex
P>>numlabs
P>> A=rand(2000, 2000, codistributor());
P>>whos
P>>size(localPart(A))
```

pmode for Interactive Parallel Computing



Outline

Scaling Up from the Desktop

- Parallel Computing Toolbox provides the ability to use up to eight local workers on a multicore or multiprocessor computer using a single toolbox license.
- When used together with MATLAB Distributed Computing Server, you can scale up your application to use any number of workers running on any number of computers.

Scaling Up from the Desktop

- Using the Configurations Manager in the toolbox, you can maintain named settings such as scheduler type, path settings, and cluster usage policies.
- Switching between clusters or schedulers typically requires changing the configuration name only.

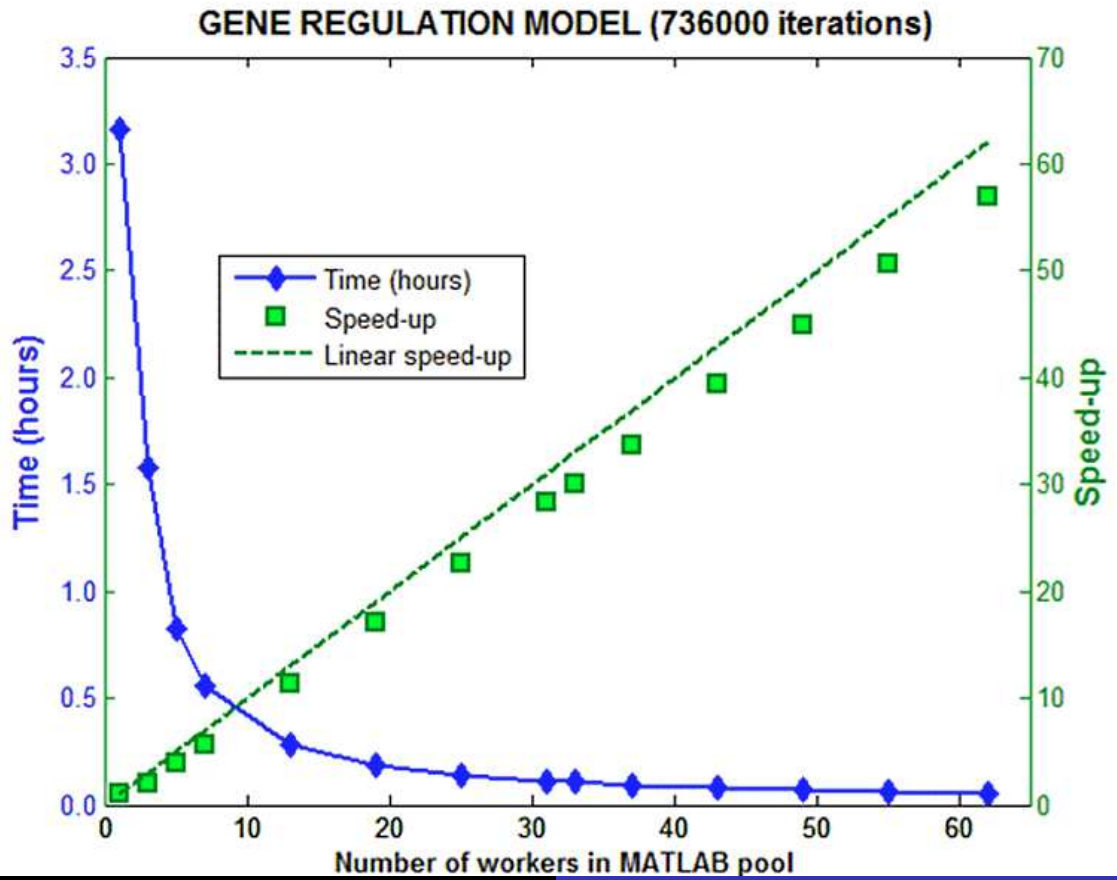
Using Parallel Configurations with PBS Pro

Parallel Configurations - Where and How the Code is Executed

- Maintain named configurations
  - Predefine cluster information and environment-specific parameters
  - No code changes required
  - Set once, use many times
- Useful for both interactive and batch workflows
- Toolbox provides GUI to manage configurations

Scaling Up from the Desktop

Example: Running a gene regulation model on a cluster using MATLAB Distributed Computing Server.



Parallel Matlab on ITC Linux Clusters

- ITC Linux Clusters
- Distriubted Computing Server Licenses for 128 workers. Users encouraged not to use more than 16 at one time.
- Matlab Configurations interface to PBS Pro for submitting jobs to the cluster
- Distributed Computing Server Licenses available on any Linux cluster that mounts /common for ITC servers
- Matlab 7.12 (with Parallel Computing Toolbox) available with full path `/common/matlab/R2011a/bin/matlab`

Running Matlab on Cluster Front-end Node

- Matlab Parallel Computing jobs can be submitted to the ITC Linux cluster by first logging onto the cluster front-end node fir.itc.virginia.edu using the NX client from your local computer and starting up Matlab from a Linux desktop terminal window.
- PCT jobs have to be submitted from within Matlab and the example scripts show how to setup and submit the jobs

Documentation: Submitting Matlab Parallel Jobs

Scripts to Launch Parallel Matlab Jobs on Cluster

- For Matlab parallel jobs where each worker runs independently of the others
  - `dist_submit2.m`
  - `myRand.m`
- For Matlab parallel jobs using the parfor command to parallelize for loops
  - `matlabpool_submit2.m`
  - `solver_large1.m`

Scripts to Launch Parallel Matlab Jobs on Cluster

- For Matlab parallel jobs that explicitly incorporate commands for the workers to communicate with each other
  - `parallel_submit2.m`
  - `colsum.m`
- Example of how to submit a Matlab parallel job and save the job id to a file so that you can log into the cluster after the job has completed and retrieve any results that were sent to the command window
  - `parallel_submit2b.m`
  - `parallel_retrieve2b.m`

Outline

GPU Computing with Matlab

MATLAB GPU Computing with NVIDIA CUDA-Enabled GPUs

ITC does not presently support GPU computing.

Outline

References

1. Mathworks Parallel Computing Toolbox Documentation
   http://www.mathworks.com/products/parallel-computing/
2. Mathworks Parallel Computing Toolbox Demos and Webinars
   http://www.mathworks.com/products/parallel-computing/demos.h
3. *Parallel Matlab for Multicore and Multinode Computers*, by Jeremy Kepner, SIAM Press.

Need further help? Email uvacse@virginia.edu.