

Introduction to High-Performance Computing

Session 06

Matlab Distributed Compute Server
(MDCS)

Introduction to MDCS

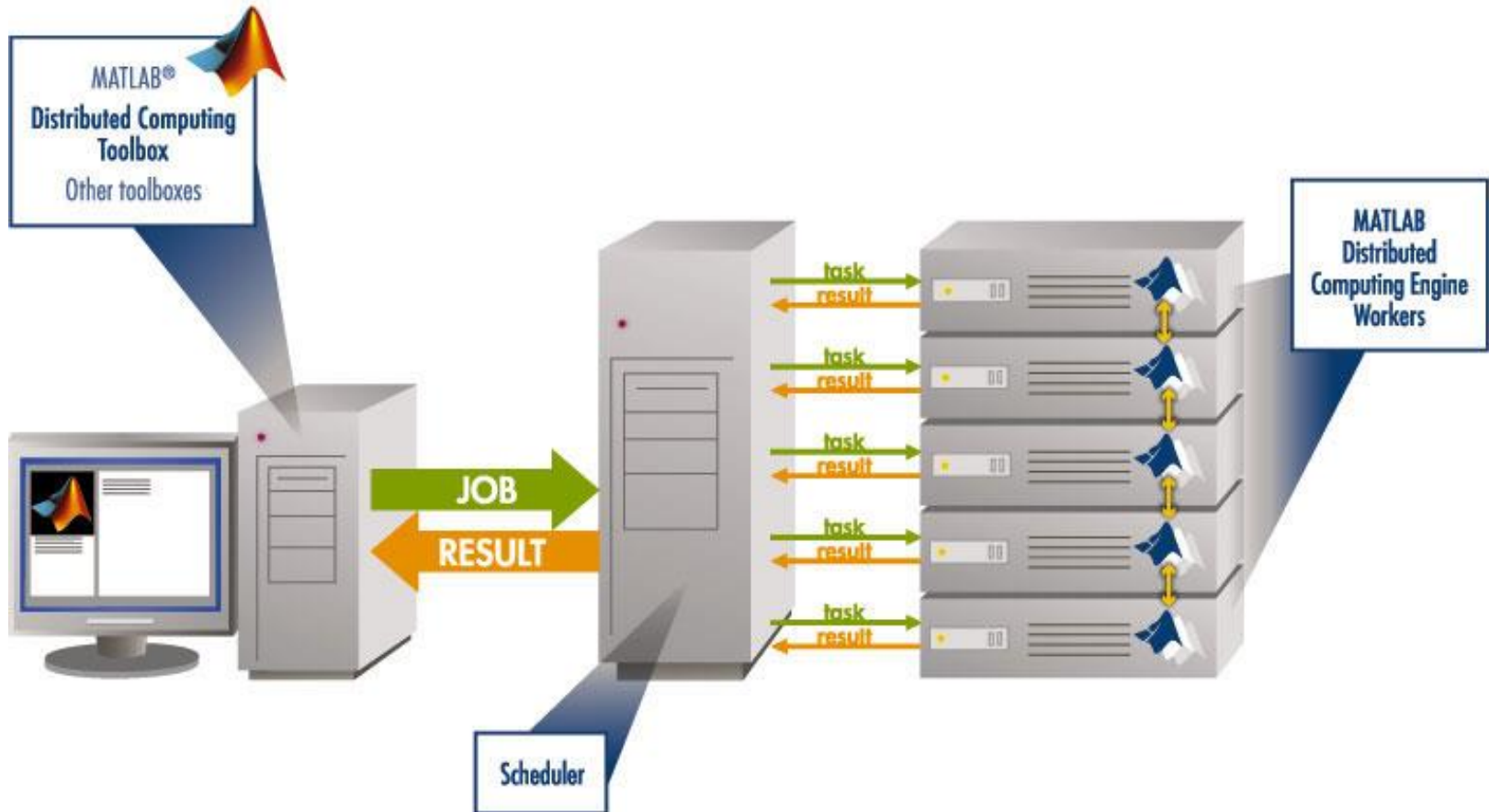
What is MDCS

Matlab on your desktop computer:

- you are limited by the compute power of your local machine
 - memory
 - CPU speed
- you can only run one job at a time
- your machine may become unusable while your Matlab job is running

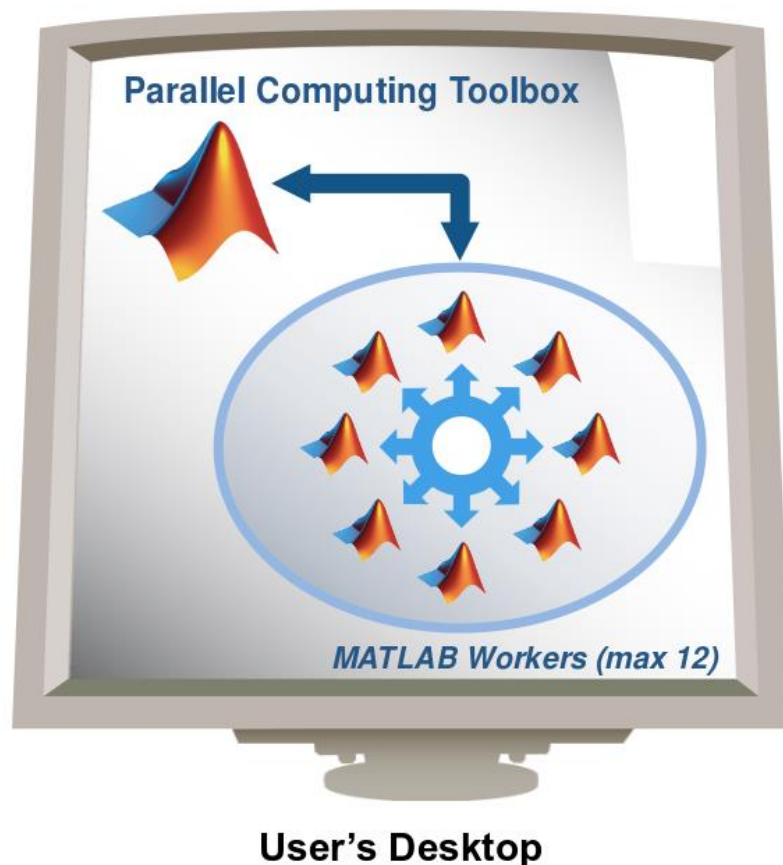


What is MDCS



Parallel Computing with Matlab

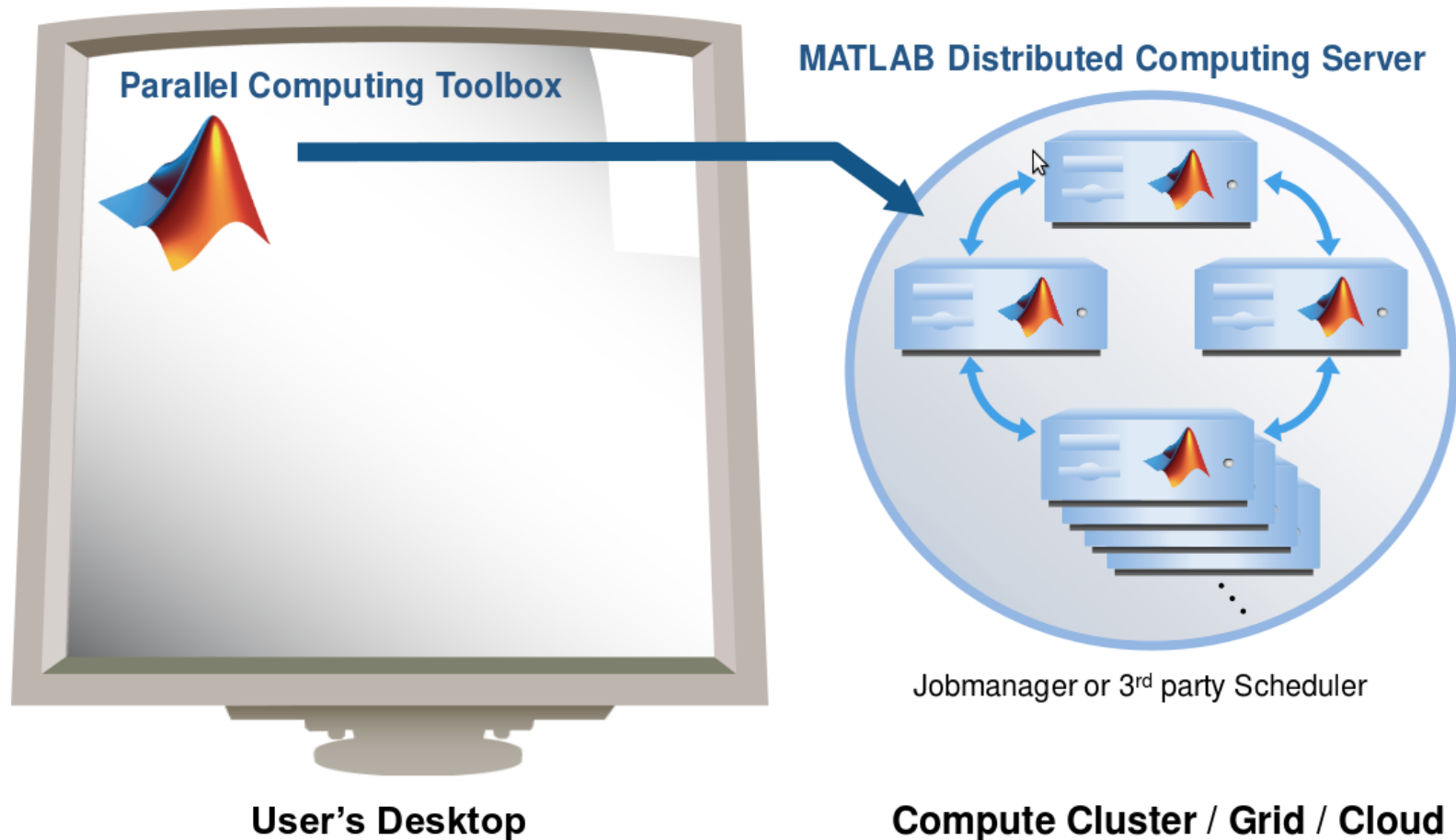
(taken from MathWorks marketing)



- easily experiment with explicit parallelism on multicore machines
- rapidly develop parallel applications on local computer
- take full advantage of desktop power, incl. GPUs
- separate compute cluster not required

Parallel Computing with Matlab

(taken from MathWorks marketing)



What is MDCS

- MDCS allows you to off-load Matlab programs to a compute server
- simplified workflow
 - you can develop and test your application locally before submitting jobs, also in parallel
 - results are automatically returned to your local machine for post-processing
- the Parallel Computing Toolbox provides utilities for parallelization
 - task-parallel
 - data-parallel

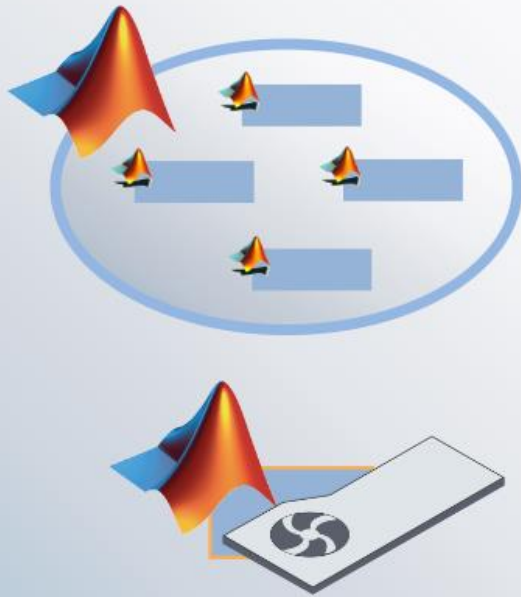
Why to use MDCS on the Cluster?

- **MDCS on the HPC cluster includes 272 worker licenses**
 - these are in addition to the normal Matlab licenses (which used to be limited to 200 for the whole university)
 - you can use also any of the toolboxes (were limited to 50)
 - allows the control over used licenses and prevents failed jobs
 - for fair sharing not more than 36 MDCS licenses should be used per job and at most two jobs per user (hard limit)
- **ease of use**
 - no need to learn about job scripts
 - work within known Matlab environment

Parallel Computing with Matlab

Larger Compute Pool

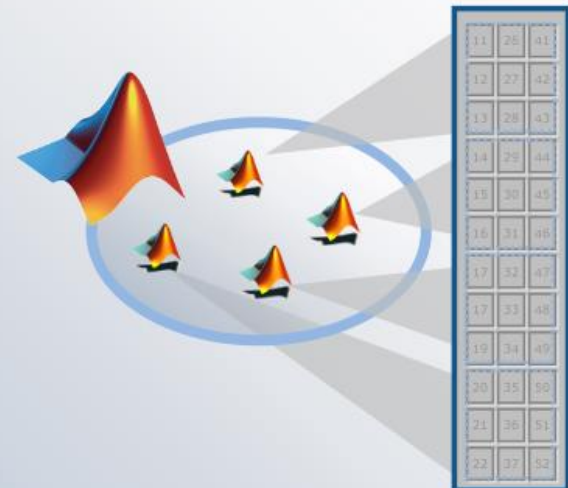
Speed up Computations



↳

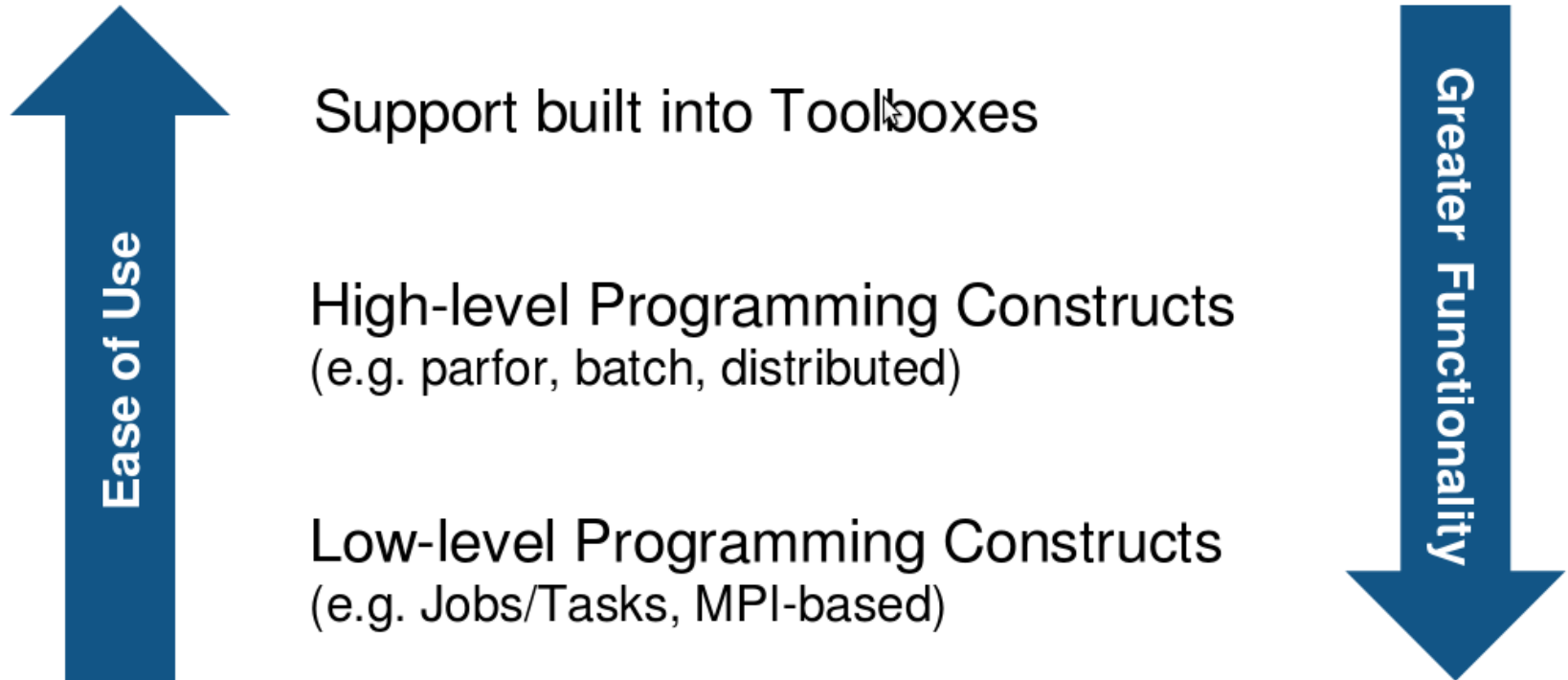
Larger Memory Pool

Work with Large Data



Parallel Computing with Matlab

Three levels of Integration:



Parallel Computing Support in Toolboxes

- Optimization Toolbox
- Global Optimization Toolbox
- Statistics Toolbox
- Simulink Design Optimization
- Bioinformatics Toolbox
- Communications Toolbox
- Model-Based Calibration Toolbox
- ... and more

see

<http://www.mathworks.com/products/parallel-computing/builtin-parallel-support.html>

Configuration of MDCS

Using MDCS on CARL/EDDY

- before you can use MDCS a few preparations are needed (**only needed to be done once**)
 - Matlab needs to be installed (see local web page) on your local machine, version must match to version on cluster (e.g. R2016b)
 - your local machine must be able to login to CARL/EDDY via ssh
 - Linux/Mac have ssh per default, for Windows you can use PuTTY
 - if you are not in the university network you also need to connect to a VPN (see HPC-Wiki for details)
 - a number of files (from a zipped archive from the HPC-Wiki) have to be copied to your local Matlab directory (depending on the setup of your local machine, your system admin has to help you)
 - a parallel configuration has to be setup with Matlab

see https://wiki.hpcuser.uni-oldenburg.de/index.php?title=Configuration_MDCS_2016

Configuration of MDCS

- login to a computer with correct version of Matlab installed

```
ssh -X hpc<nn>@134.106.219.162
```

```
– password: _hpc$17<nn>_
```

```
– replace <nn> with 01, 02, .. or 08
```

- start Matlab

```
matlab &
```

```
– maybe slow
```

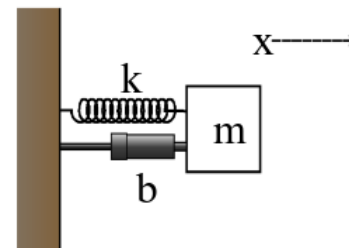
```
– server configuration is already done
```

```
– add user configuration for your university account
```

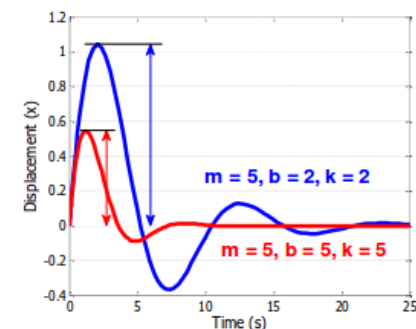
Using MDCS on CARL/EDDY

- once you have completed the setup you can submit jobs to the cluster
 - example parameter sweep for 2nd-order ODE (taken from the [HPC-Wiki](#))
 - dampened oscillator

$$\overbrace{m}^5 \ddot{x} + \underbrace{b}_{1,2,\dots} \dot{x} + \underbrace{k}_{1,2,\dots} x = 0$$



- simulate with different values for b and k
- record peak value for each run



2nd-order ODE for example

odesystem.m

```
function dy = odesystem(t, y, m, b, k)
% 2nd-order ODE
%
%  $m \cdot X'' + b \cdot X' + k \cdot X = 0$ 
%
% --> system of 1st-order ODEs
%
%  $y = X'$ 
%  $y' = -1/m * (k \cdot y + b \cdot y')$ 
% Copyright 2009 The MathWorks, Inc.

dy(1) = y(2);
dy(2) = -1/m * (k * y(1) + b * y(2));

dy = dy(:); % convert to column vector
```


Parameter Sweep: serial Matlab code

paramSweep_batch.m

```
%% Initialize Problem
m      =      5; % mass
bVals  = 0.1:.1:15; % damping values (step .1)
kVals  = 1.5:.1:15; % stiffness values (step .1) damping
[kGrid, bGrid] = meshgrid(bVals, kVals);
peakVals = nan(size(kGrid));

%% Parameter Sweep
tic;

for idx = 1:numel(kGrid)
    % Solve ODE
    [T,Y] = ode45(@(t,y) odesystem(t, y, m, bGrid(idx), kGrid(idx)), ...
        [0, 25], ... % simulate for 25 seconds
        [0, 1]); % initial conditions

    % Determine peak value
    peakVals(idx) = max(Y(:,1));
end

t1 = toc;
```

Parameter Sweep: parallel Matlab code

paramSweep_batch.m

```
%% Initialize Problem
m      =      5; % mass
bVals  = 0.1:.1:15; % damping values (step .1)
kVals  = 1.5:.1:15; % stiffness values (step .1) damping
[kGrid, bGrid] = meshgrid(bVals, kVals);
peakVals = nan(size(kGrid));

%% Parameter Sweep
tic;

parfor idx = 1:numel(kGrid)
    % Solve ODE
    [T,Y] = ode45(@(t,y) odesystem(t, y, m, bGrid(idx), kGrid(idx)), ...
        [0, 25], ... % simulate for 25 seconds
        [0, 1]); % initial conditions

    % Determine peak value
    peakVals(idx) = max(Y(:,1));
end

t1 = toc;
```

Using MDCS on CARL/EDDY

- submitting jobs to the cluster

```
 sched = parcluster('CARL');  
 job = batch(sched, 'paramSweep_batch', 'Pool', 7, ...  
             'AttachedFiles', {'odesystem.m'});
```

- first command creates a handle for the cluster using the available configuration
- second command creates a job and sends it to the cluster
 - Matlab script is executed on the cluster
 - requests a pool of workers (number of processes is +1 for master)
 - uses default resources unless modified
 - files can be attached but Matlab also automatically attaches needed files (if it can find them and if not disabled)

Using MDCS on CARL/EDDY

- changing resource allocation

```
set(sched, 'CommunicatingSubmitFcn',  
    cat(2, sched.CommunicatingSubmitFcn,  
        {'runtime', '72:0:0', 'memory', '4G'}));
```

- changes maximum runtime and memory per worker
- path-dependency as alternative to attaching files
 - use addpath within script (.m-files)
 - use AdditionalPath property of scheduler object
 - use absolute path names
 - copy files to the cluster before submitting job

Using MDCS on CARL/EDDY

- recovering jobs
 - it is possible to terminate the local Matlab session while jobs are running (or waiting on the cluster)
 - to reconnect

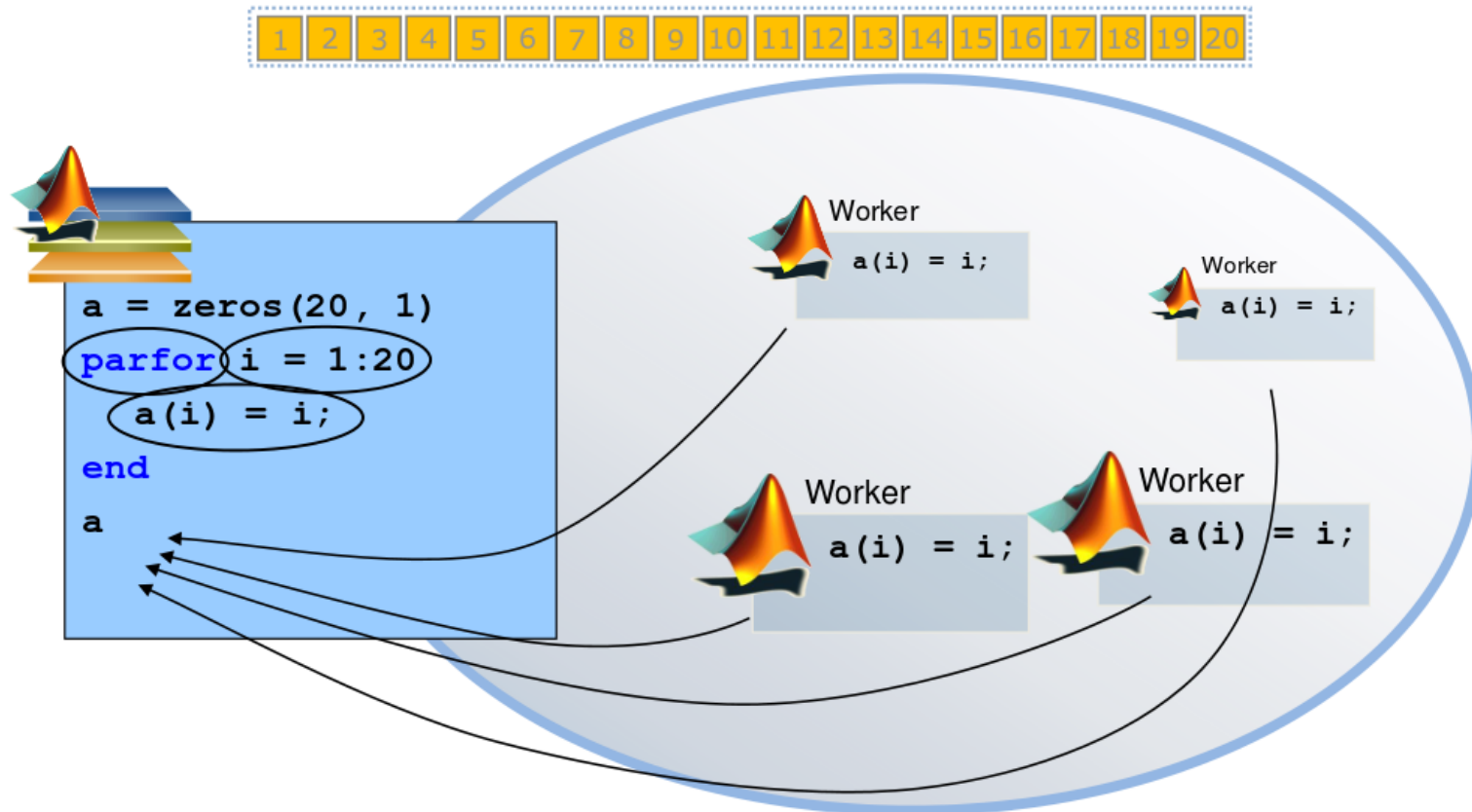
```
sched = parcluster('HERO');  
sched.Jobs % to list available jobs  
job = sched.Jobs(1) % to get job information  
jobData = load(job);
```

Monitoring Jobs and Error Tracking

- Matlab Job Monitor for basic information
- use `squeue` and `sacct` for additional information from SLURM
- job handle can be used to get information about errors
- Matlab diary for additional log output
- files in the job directory

MDCS with parfor

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`)
 - cannot contain `break` or `return` statements
 - cannot contain another `parfor` loop

Variable Classification

- all variables referenced at the top level of the **parfor** must be resolved and classified

Classification	Description
loop	serves as a loop index for arrays
sliced	an array whose segments are operated on by different iterations
broadcast	a variable defined before the loop whose value is used inside the loop, but never assigned in 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

- matrix-vector multiplication

```
N=2048;                                % N is broadcast  
b=rand(N,1);                            % b is broadcast  
A=rand(N,N);                            % A is slices input  
  
parfor i=1:N                            % i is loop index  
    c(i)=A(i,:)*b(:);                    % c is sliced output  
end
```

parfor Examples

- this example cannot be parallized in **parfor**

```
j=zeros(100);      %pre-allocate vector
j(1)=5;
for i=2:100;
    j(i)=j(i-1)+5;
end;
```

- order of iterations is important

parfor Examples

- functions with multiple output may confuse Matlab

```
for i=1:10
    [x{i}(:,1), x{i}(:,2)]=functionName(z,w);
end;
```

- use this instead

```
for i=1:10
    [x1, x2]=functionName(z,w);
    x{i}=[x1 x2];
end;
```

parfor Considerations

- **parfor** often only involves minimal code changes
- if a for loop cannot be converted to **parfor**, consider wrapping a subset of loop body in a function
 - e.g. `load` works not in **parfor**, however it does work in function that is called inside a **parfor** loop
- more information
<http://blogs.mathworks.com/loren/2009/10/02/using-parfor-loops-getting-up-and-running/>
- there is a Code-Analyzer to diagnose **parfor** issues

MDCS with spmd (single program multiple data)

SPMD

	Client			Worker 1			Worker 2					
	a	b	e		c	d	f		c	d	f	

a = 3;	3	-	-		-	-	-		-	-	-	
b = 4;	3	4	-		-	-	-		-	-	-	
spmd												
c = labindex();	3	4	-		1	-	-		2	-	-	
d = c + a;	3	4	-		1	4	-		2	5	-	
end												
e = a + d{1};	3	4	7		1	4	-		2	5	-	
c{2} = 5;	3	4	7		1	4	-		5	6	-	
spmd												
f = c * b;	3	4	7		1	4	4		5	6	20	
end												

SPMD

- when a SPMD block ends the workspace is saved, the worker is paused
- data is preserved from one block to the next
- does not apply to SPMD block in a function after the function is completed (as regular variables local to a function)

SPMD Example

```
x = imread ( 'balloons.tif' );  
y = imnoise ( x, 'salt & pepper', 0.30 );  
yd = distributed ( y );  
  
spmd  
    yl = getLocalPart ( yd );  
    yl = medfilt2 ( yl, [ 3, 3 ] );  
end  
  
z(1:480,1:640,1) = yl{1};  
z(1:480,1:640,2) = yl{2};  
z(1:480,1:640,3) = yl{3};
```

- read image
- add noise to image
- distribute data
- parallel working on image data (filter)
- on master process put together filtered image



Distributed Data

- Matlab provides different functions to manage distributed data
 - with `distributed(X)` you can distribute data among workers
 - with `distributed.METHOD` you can create data distributed among workers
 - workers can create codistributed data structures which become distributed data outside of the SPMD block
 - a datastore can be distributed to read manage large data files with multiple workers
 - see ‘help distributed’ for more information

SPMD Example

- increase contrast of an image

```
%  
% Read an image  
%  
x = imageread( 'surfsup.tif' );  
%  
% Since the image is black and white, it will be distributed by columns  
%  
xd = distributed(x);  
%  
% Each worker enhances the contrast on its portion of the picture  
%  
spmd  
    xl = getLocalPart(xd);  
    xl = nlfilter( xl, [3, 3], @adjustContrast);  
    xl = uint8(xl);  
end  
%  
% Concatenate the submatrices to assemble the whole image  
%  
xf_spmd = [ xl{:} ];
```

SPMD Example

- algorithm produces artifacts when parallelized on multiple workers
- problem is that increasing contrast requires information from neighbouring pixel
- distributing the data adds additional boundaries

Filtered on Client

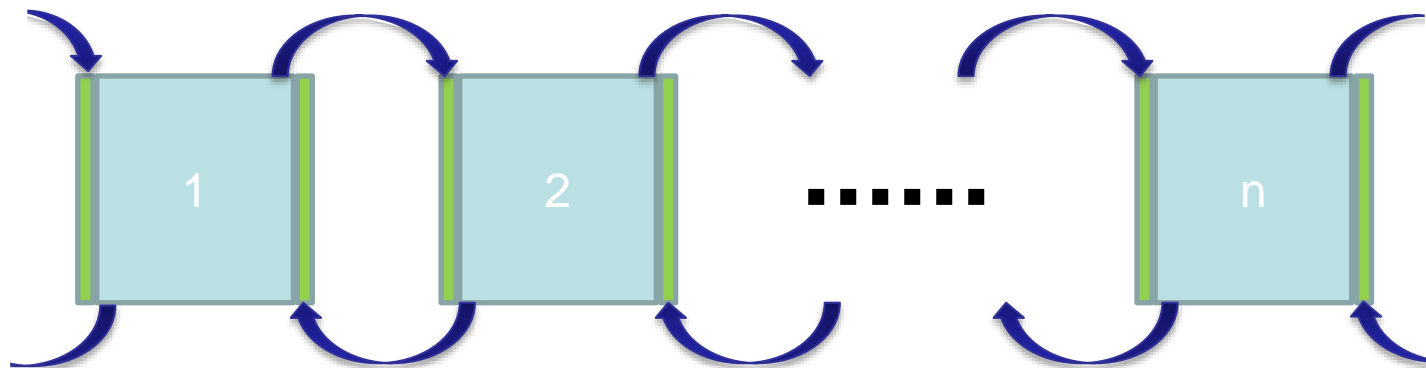


Filtered on 4 SPMD Workers



labSendReceives

- solution is communication between workers
 - each worker has to send one boundary left and one right
 - each worker has to receive one boundary from left and one from right
 - extra columns are added before filter is applied, and need to be removed again afterwards



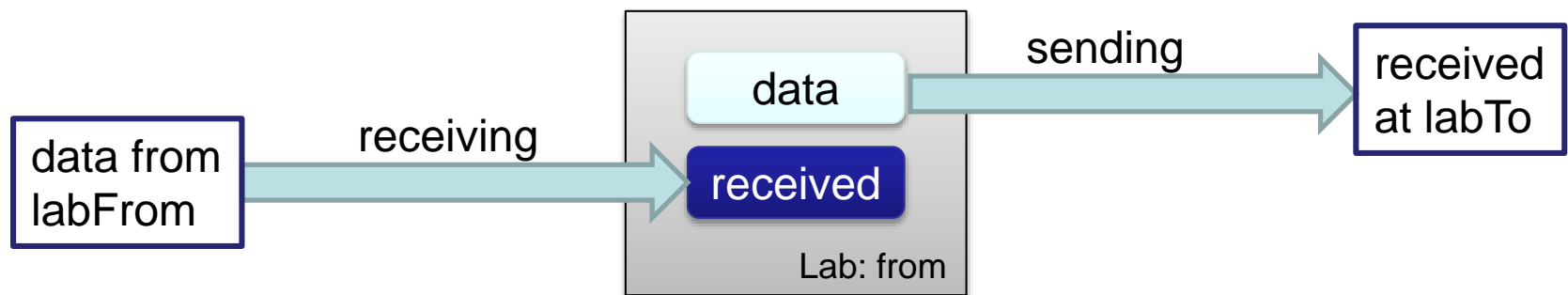
labSendReceives

- the function `labSendReceive` simultaneously sends and receives data

```
received = labSendReceive (labTo, labFrom, data)
```

- sends data to `labTo`

- receives data from `labFrom` and stores it in `received`



labSendReceive

```
column = labSendReceive ( previous, next, x1(:,1) );

if ( labindex() < numlabs() )
    x1 = [ x1, column ];
end

column = labSendReceive ( next, previous, x1(:,end - 1) );

if ( 1 < labindex() )
    x1 = [ column, x1 ];
end
```


Heat Example in Matlab

```
% 2d-heat example in Matlab
% initial setup
NXPROB = 20;           % number of grid rows
NYPROB = 20;           % number of grid columns
STEPS   = 100;         % number of iterations
TIME    = 0;           % initial and current time

uvals = zeros(2, NXPROB, NYPROB); % allocate grid
uvals = inidat(uvals);           % initialize grid

plotdat(uvals, 1, TIME);         % make plot

it = 1;
for TIME=1:STEPS                 % time iteration
    uvals = updateu(uvals, it);   % update thermal energy
    it    = 3 - it;
end

plotdat(uvals, 1, TIME);         % make plot
```