Introduction to High-Performance Computing

Session 08

Matlab Distributed Compute Server (MDCS)

Questions

- Are you already using Matlab?

  a) Yes, on my own/work computer
  b) Yes, and I am already using the HPC cluster
  c) No, not yet

Questions

- Did you install Matlab on the computer you are using now?

a) Yes, Matlab R2019b
b) Yes, Matlab R2018b
c) Yes, another version
d) No

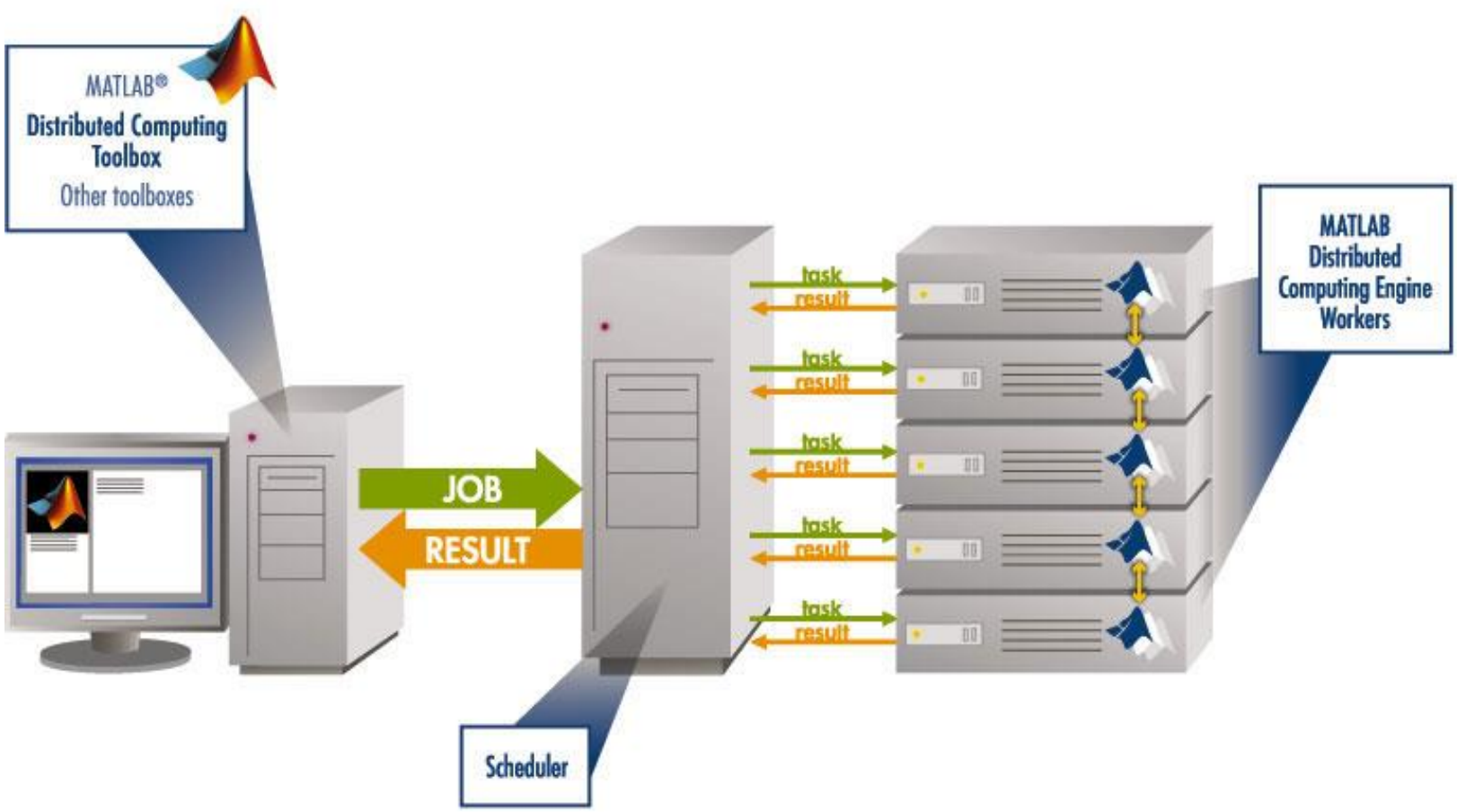
Introduction to MDCS

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


MATLAB®
Distributed Computing Toolbox
Other toolboxes
JOB
RESULT
task
result
task
result
task
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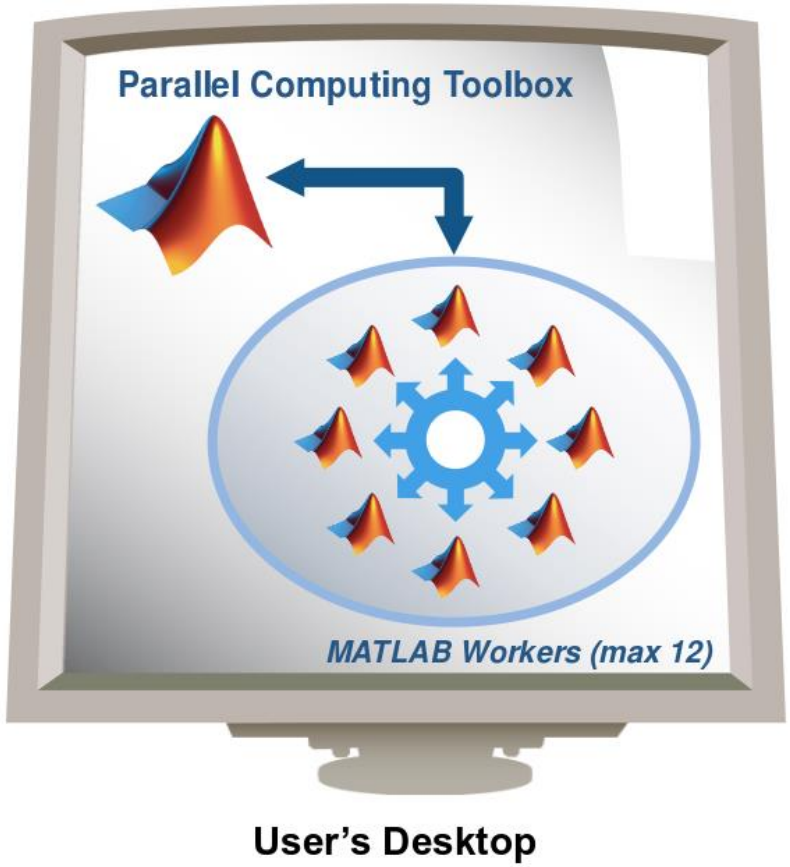
task
result
task
result
MATLAB Distributed Computing Engine Workers
Scheduler

Parallel Computing with Matlab

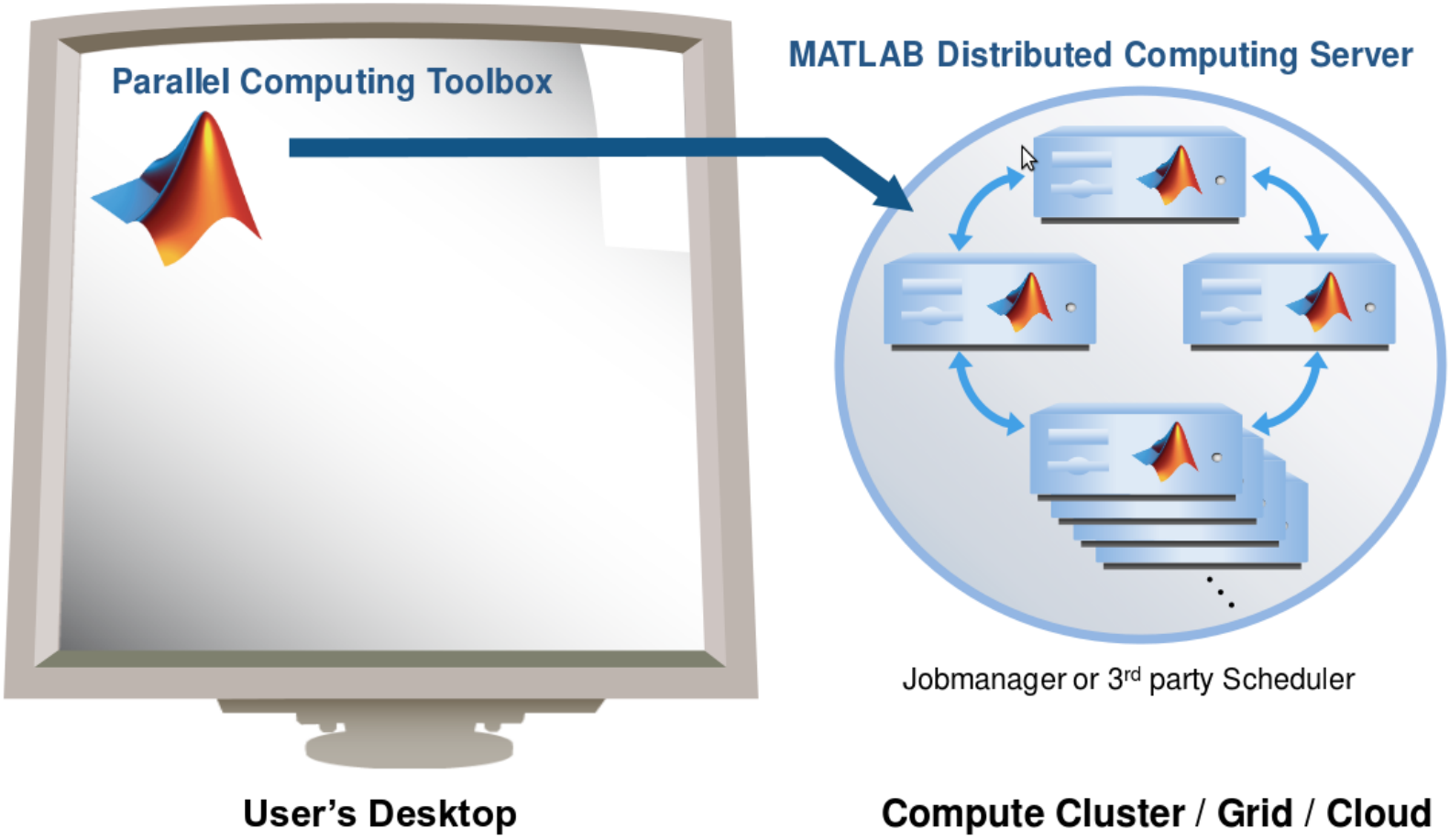
(taken from MathWorks marketing)



- 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?

- easy to use
  - work on your local computer within known Matlab environment
  - files (scripts, data, results) are automatically transfered
  - no need to learn about job scripts (but it helps to know a little)

- parallelization across multiple nodes
  - make use of distributed memory
  - use parallel threads (CPU cores) for each worker

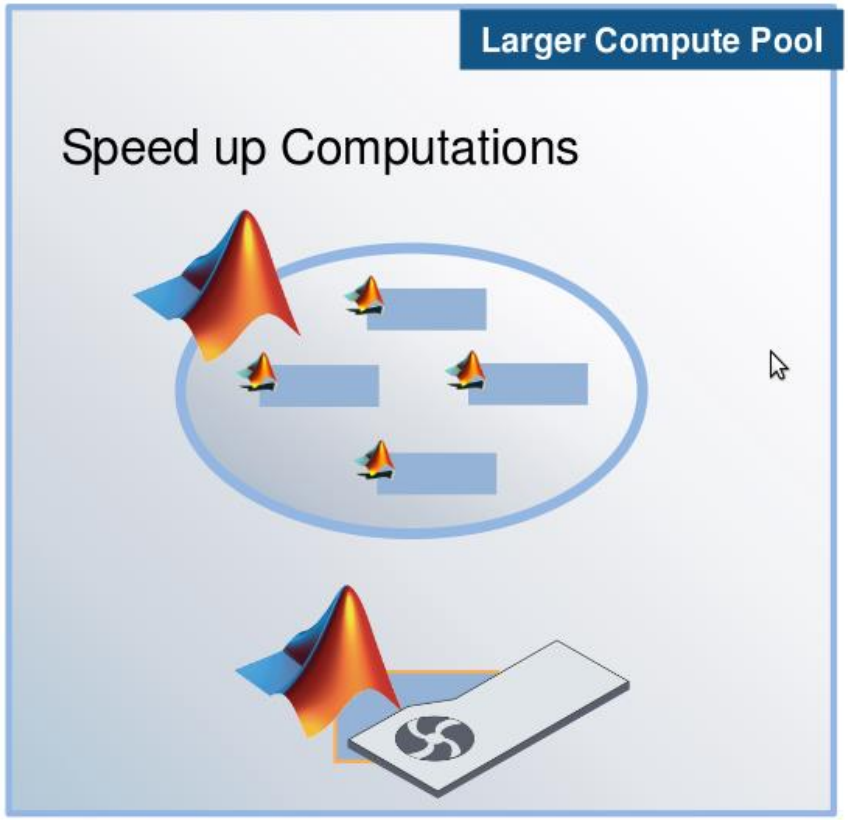
```
>> maxNumCompThreads(1);     % set the number of threads to 1
>> a = rand(4096); b = rand(4096);  % create to matrices
>> tic;c=a*b;toc             % compute and time matrix multiplication
Elapsed time is 3.633846 seconds.
>> maxNumCompThreads(4);     % set the number of threads to 4
>> tic;c=a*b;toc             % compute and time matrix multiplication
Elapsed time is 1.019613 seconds.
>> maxNumCompThreads('automatic');     % set the number of threads to automatic
>> tic;c=a*b;toc             % compute and time matrix multiplication
Elapsed time is 0.257363 seconds.
```

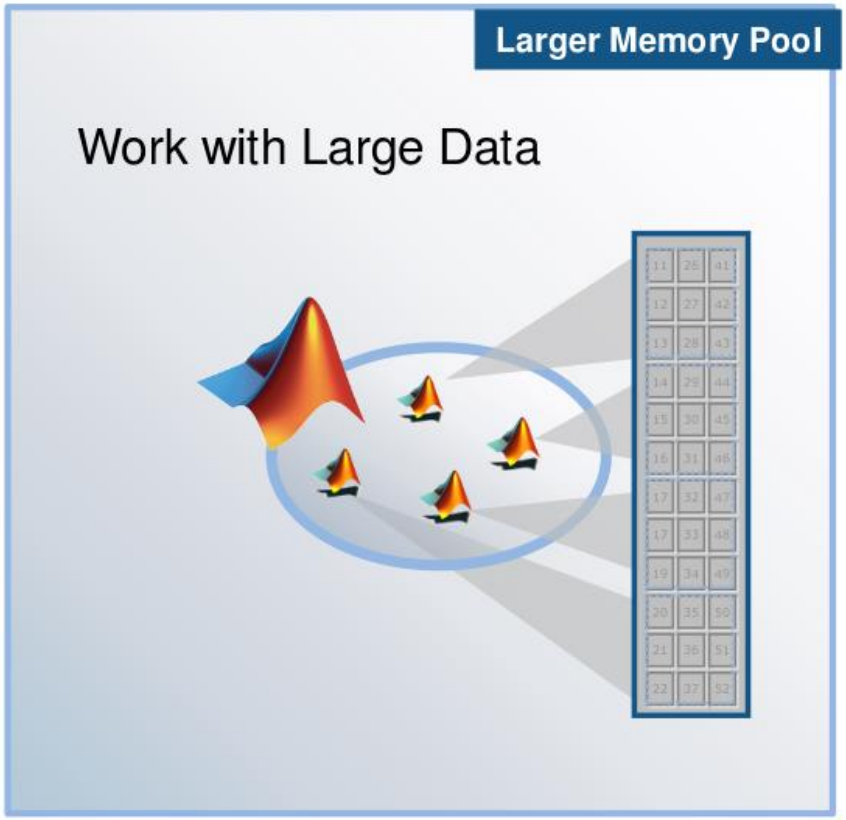
MDCS Licenses

- MDCS on the HPC cluster includes 272 worker licenses
  - Matlab used to be limited to 200 licenses, now Campus license
  - for fair sharing not more than 36 MDCS licenses should be used per job and at most two jobs per user (hard limit)
  - check license use on the cluster:

```
[abcd1234@carl]$ scontrol show license mdcs
LicenseName=mdcs
    Total=272 Used=47 Free=225 Remote=no
```

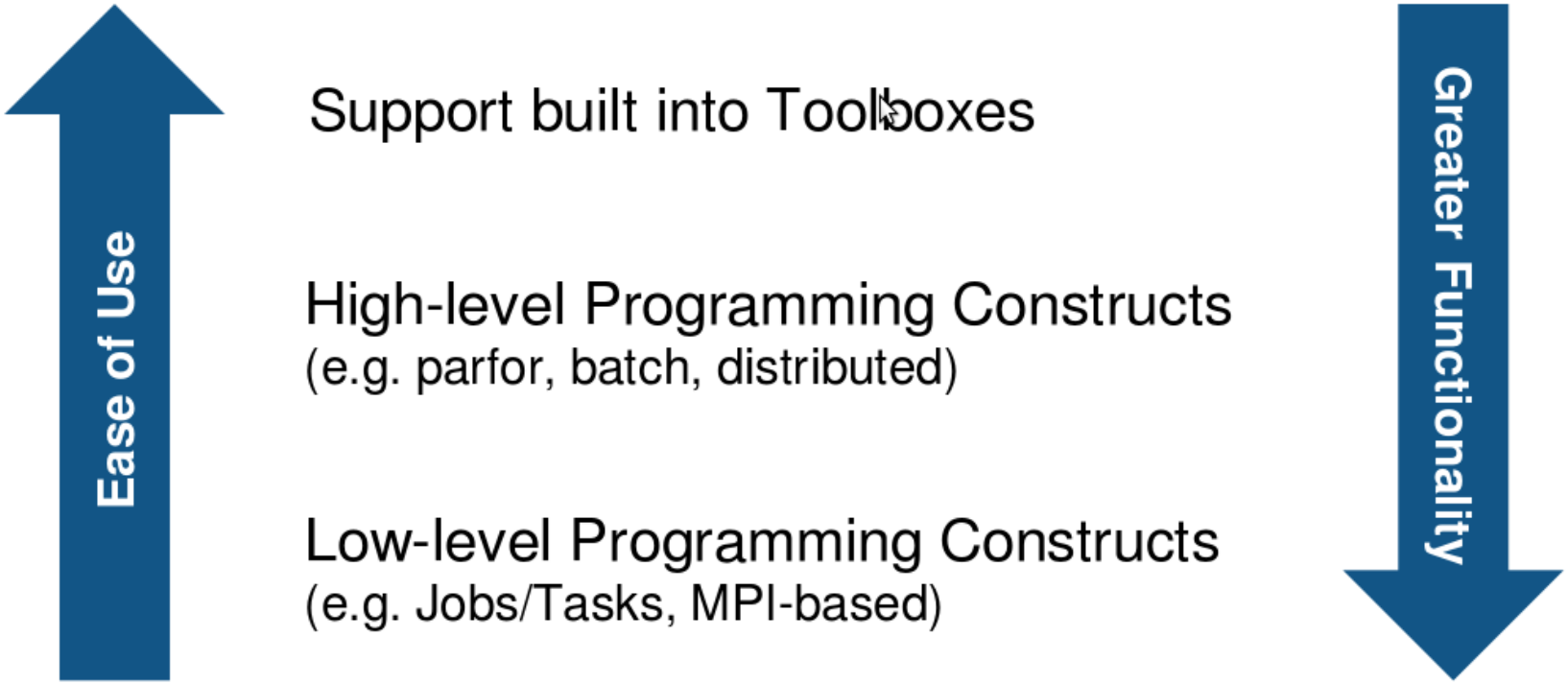
Parallel Computing with Matlab





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 Cluster Profile

- the remote system is described in the cluster profile

`JobStorageLocation`:	local directory for job data, e.g. **`C:\Users\name\Documents\MATLAB\2019b\JobData`**
`RemoteJobStorageLocation`:	local directory for job data, e.g. on **`$WORK`** **`/gss/work/abcd1234/MATLAB/2019b/JobData`**

  - directories are sync'd at job submission and after the job has completed
  - existing workspace is copied at job submission (can affect submission time)
  - workspace of main process is copied back (can affect job load time), use e.g. **`clear bigvar1 bigvar2;`** (and save in separate files if needed)

Configuration of MDCS Cluster Profile

- the remote system is described in the cluster profile

`JobStorageLocation`:	local directory for job data, e.g. **`C:\Users\name\Documents\MATLAB\2019b\JobData`**
`RemoteJobStorageLocation`:	local directory for job data, e.g. on **`$WORK`** **`/gss/work/abcd1234/MATLAB/2019b/JobData`**
`NumWorkers`:	set to 36 for fair sharing
`NumThreads`:	set to 1 (default), can be changed when useful

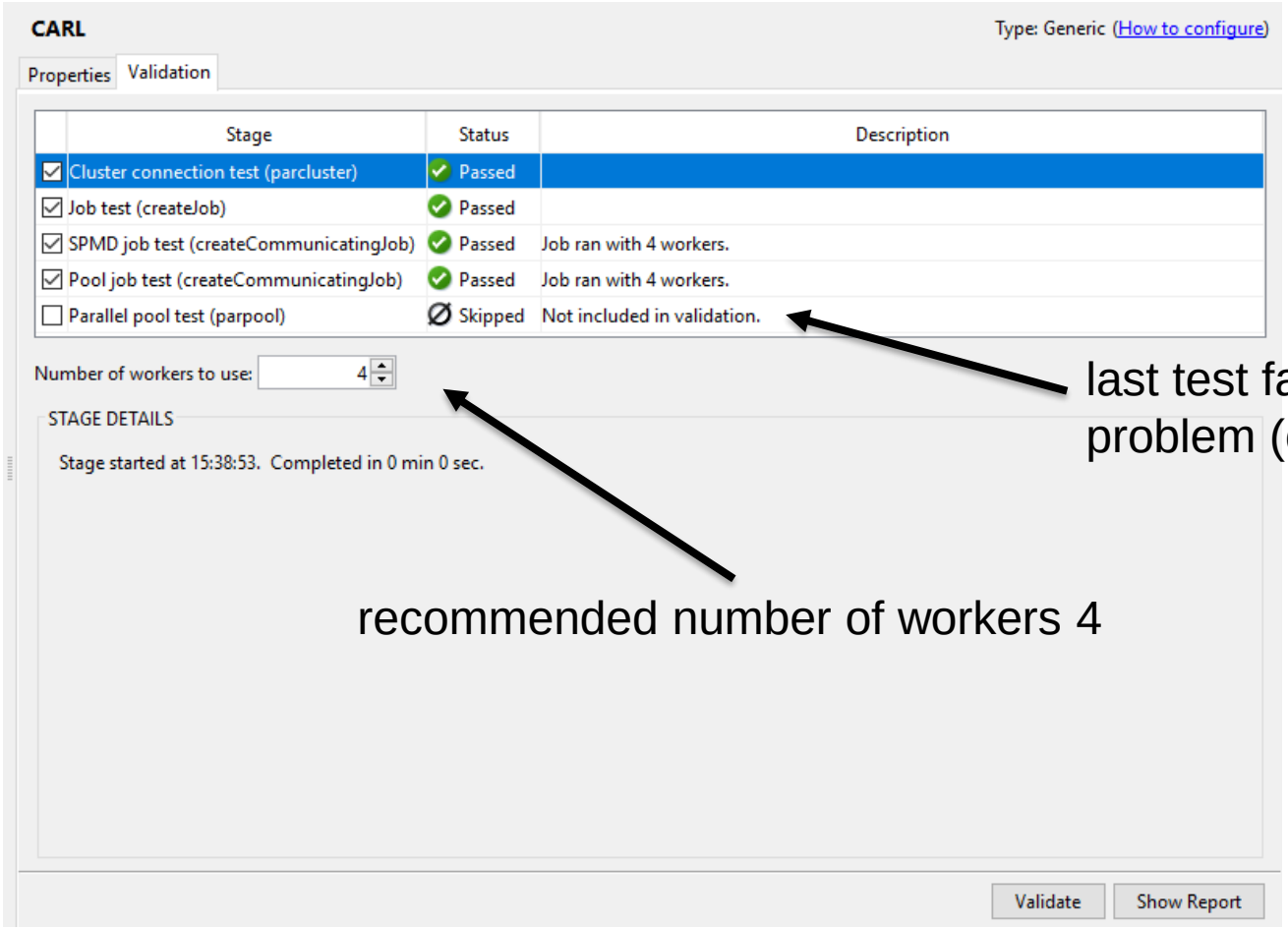
  - change with e.g.: **`sched.NumThreads=4;`**
  - maximum number of threads is the number of CPU cores in a node
  - total number of cores allocated is **`(worker+1)*NumThreads`**
  - benchmark your code to determine a good number of threads per worker.

Configuration of MDCS Cluster Profile

- the remote system is described in the cluster profile

`JobStorageLocation`:	local directory for job data, e.g. **`C:\Users\name\Documents\MATLAB\2019b\JobData`**
`RemoteJobStorageLocation`:	remote directory for job data, e.g. on **`$WORK`** **`/gss/work/abcd1234/MATLAB/2019b/JobData`**
`NumWorkers`:	set to 36 for fair sharing
`NumThreads`:	set to 1 (default), can be changed when useful
`AdditionalProperties`:	set at least **`ClusterHost`** and **`RemoteJobStorageLocation`** (see above), addtional options for password-free login are described in HPC wiki

Validation of MDCS Cluster Profile



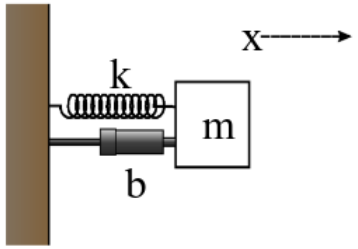
last test fails but that is not a problem (can be skipped)

recommended number of workers 4

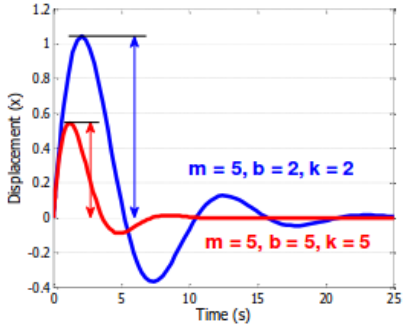
Using MDCS on CARL/EDDY

- 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

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



  - 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*X'' + b*X' + k*X = 0
%
% --> system of 1st-order ODEs
%
%   y  = X'
%   y' = -1/m * (k*y + b*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

```
sched.AdditionalProperties.runtime='0:30:00';
sched.AdditionalProperties.memory='4G';
remove(sched.AdditionalProperties, 'memory');
```

  - changes maximum runtime and memory per worker
  - remove previous setting to get default
  - older Matlab versions use a different format (see HPC wiki)

- 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

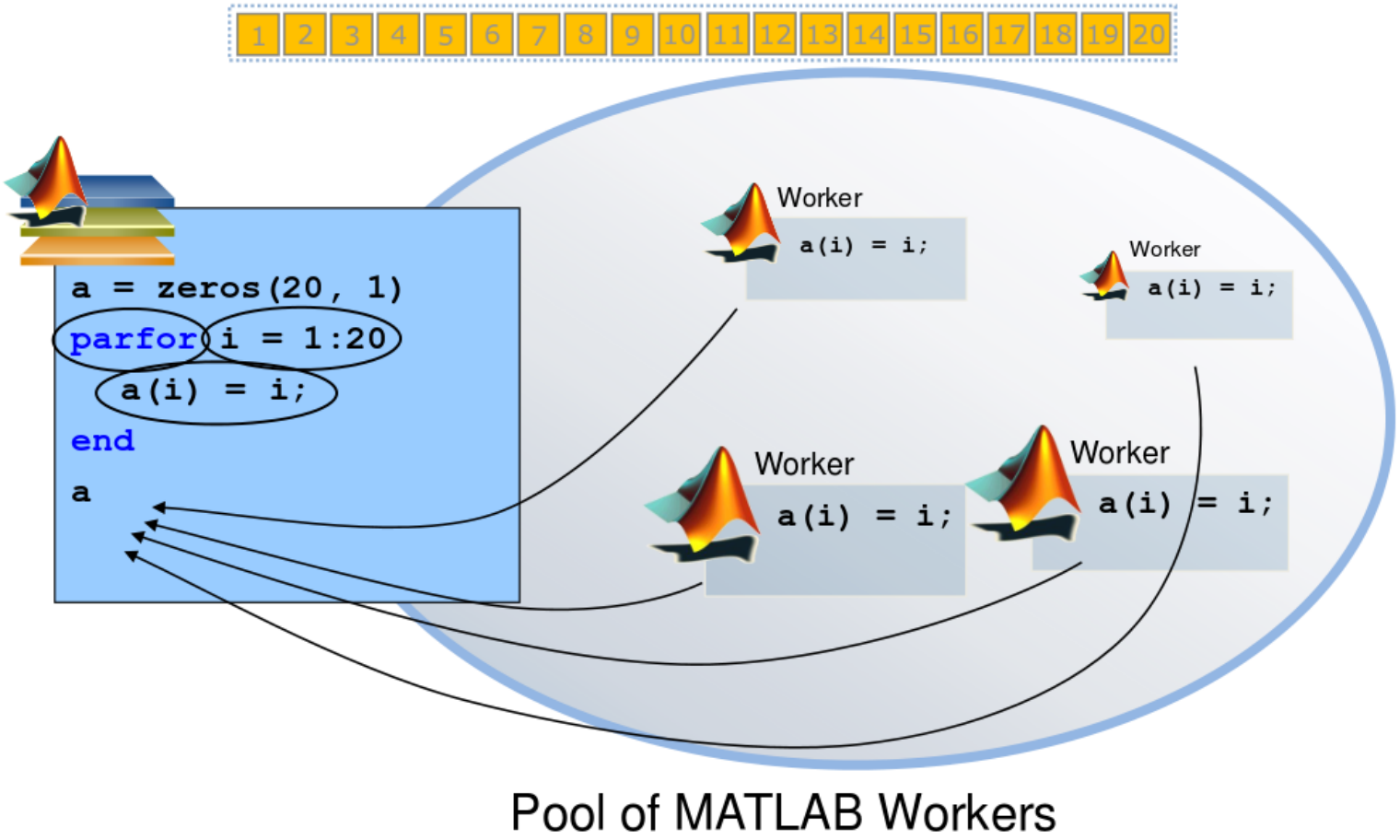
```
sched   = parcluster(,CARL');
sched.Jobs   % to list available jobs
job     = sched.Jobs(1)   % to get job information
jobData = load(job);
```

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



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

https://de.mathworks.com/help/parallel-computing/troubleshoot-variables-in-parfor-loops.html

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` Examples

- be careful not to broadcast unnecessary data

```
data.raw = ...
data.processed = ...

% Inefficient variant:
parfor idx = 1 : N
    % do something with data.processed
end

% This is better:
processedData = data.processed;
parfor idx = 1 : N
    % do something with processedData
end
```

https://undocumentedmatlab.com/blog/a-few-parfor-tips

`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

Distributed Data

distributing data from client

```
p = parpool('local', 4);      % create a local pool of workers
A = zeros(4);                 % create a 4x4 matrix with zeros
A                             % print A on client
B = distributed(A);           % distribute A to the workers
spmd                          % begin parallel spmd region
    B = B + labindex;         % modify distributed data in B
end                           % end parallel spmd region
B                             % print B on client
delete(p);
```

vs.

codistributed data created on workers

```
p = parpool('local', 4);                        % create a pool of workers
spmd                                            % begin parallel spmd region
    codist = codistributor1d(2, [1,1,1,1]); % define distribution
    B = zeros(4, codist);                       % created codistributed array
    B = B + labindex;                           % modify distributed data in B
end                                             % end parallel spmd region
B                                               % print B on client
delete(p);
```

Example: Image Contrast

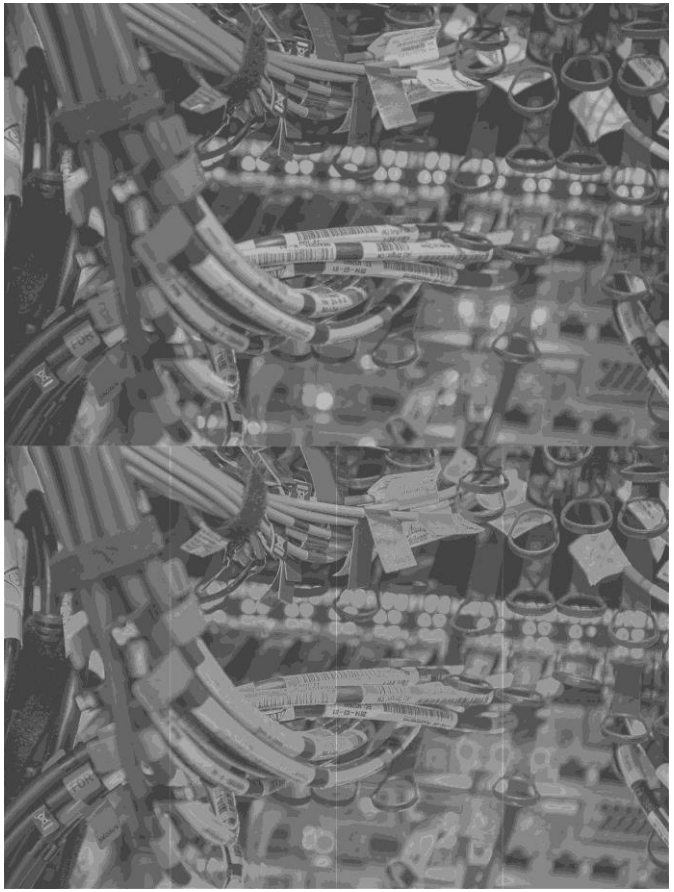
- a Matlab script that uses a simple function to change the contrast of an gray-scale image

```
% read an image (gray-scale)
y = imread('low_contrast.jpg');

% setup function for contrast manipulation
c = 1.7;
adjustContrast = @(x) c*x(2,2)+(1.0-c)*(mean(x(:)-x(2,2)/9.0));

% apply filter
z = nlfilter(y, [3,3], adjustContrast);

% save image side-by side
imwrite(cat(1,y,z), 'contrast_serial.jpg');
```

Example: Image Contrast

- parallelize with SPMD

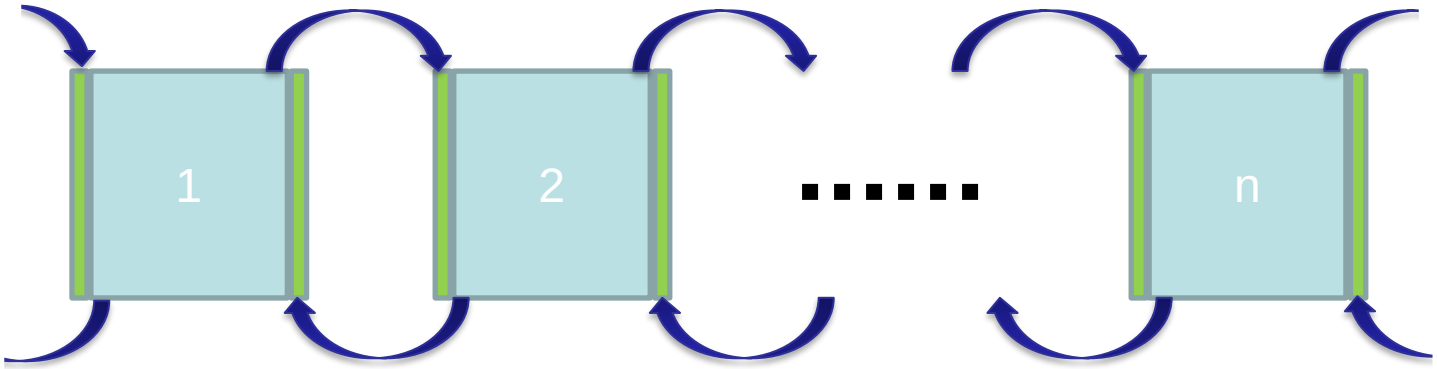
```
% read an image (gray-scale)
y = imread('low_contrast.jpg');

% setup function for contrast manipulation
c = 1.7;
adjustContrast = @(x) c*x(2,2)+(1.0-c)*(mean(x(:)-x(2,2)/9.0));

% distribute image by columns
yd = distributed(y);

% now work in parallel
spmd
    yl = getLocalPart(yd);

    % apply filter
    yl = nlfilter(yl, [3,3], adjustContrast);

end

% combine local images
z = [ yl{:}];

% save image side-by side
imwrite(cat(1,y,z), 'contrast_spmd.jpg');
```



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

labSendReceive

- solution is communication between workers
  - each worker has to sent 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

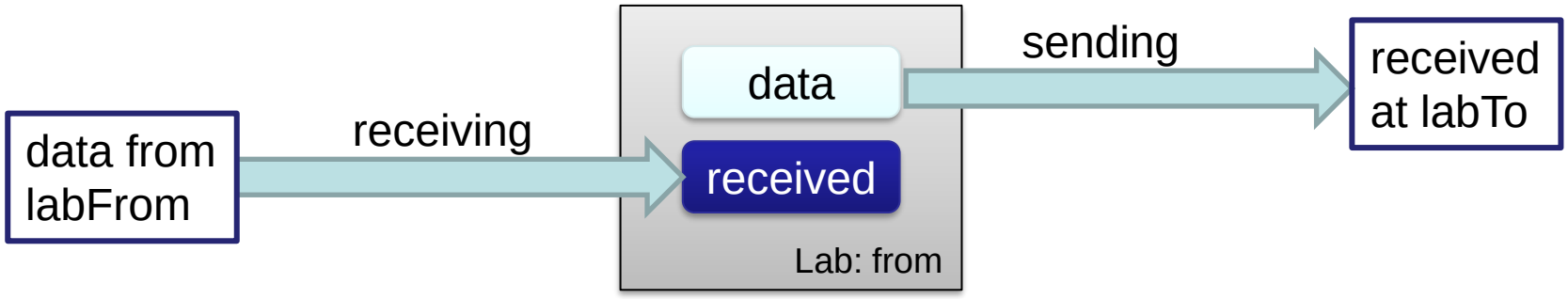


labSendReceive

- 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, xl(:,1) );

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

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

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

Exercise: 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
```