

# WORKSHOP: Parallel Computing With MATLAB (Part II)





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# Agenda

- Part I Parallel Computing with MATLAB on the Desktop
  - Parallel Computing Toolbox
- Part II Scaling MATLAB to the TRUBA HPC cluster
  - MATLAB Parallel Server





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- Part I Parallel Computing with MATLAB on the Desktop
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# Simply Complex Lab: Scaling with MATLAB Parallel Server

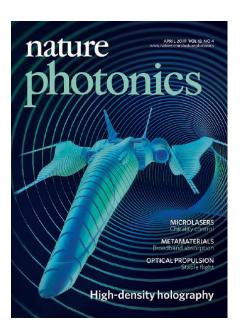


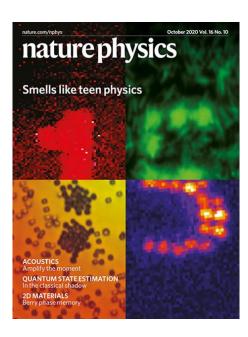




Simply Complex Lab is driven towards deciphering emergent, complex, far from equilibrium phenomena. We are determined to solve scientifically and technologically persistent problems by exploring solutions under far from equilibrium conditions. Such conditions dictate:

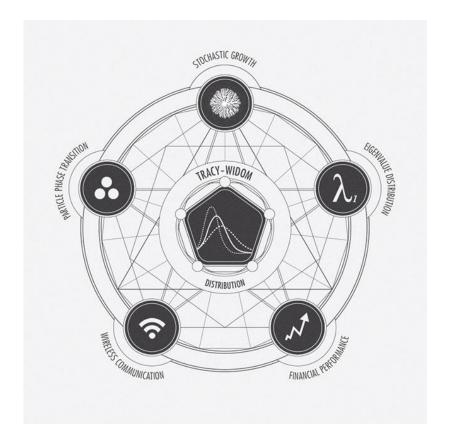
- sufficiently high nonlinearity
- strong stochasticity
- intrinsic positive and negative feedback mechanisms

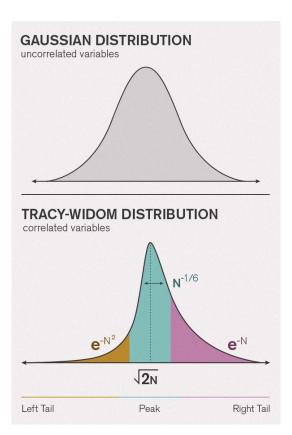


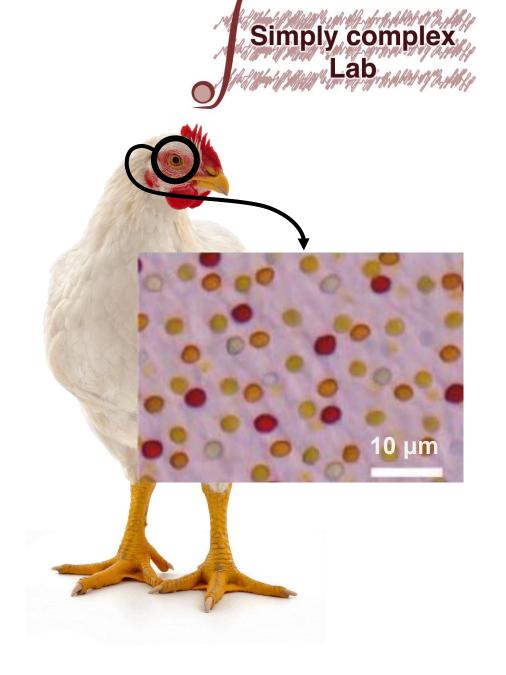


The group's work was highlighted on the covers of Nature photonics and Nature Physics journals





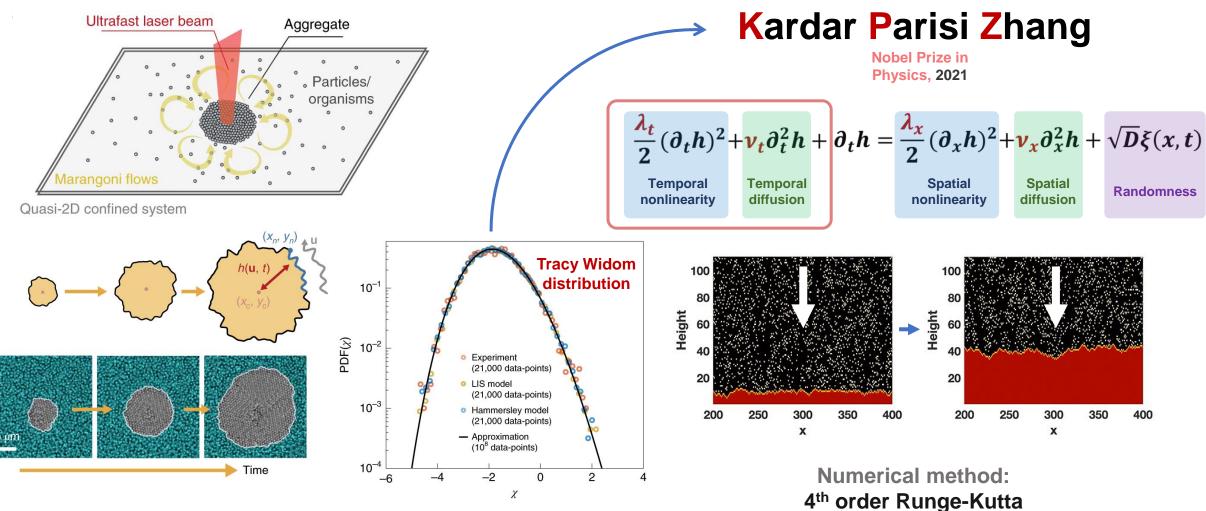




"At the Far Ends of a New Universal Law," Quantum Magazine





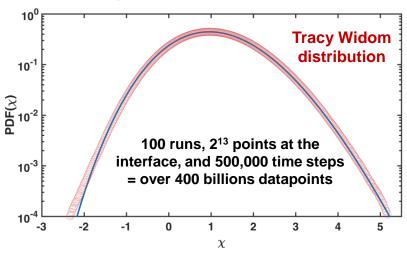


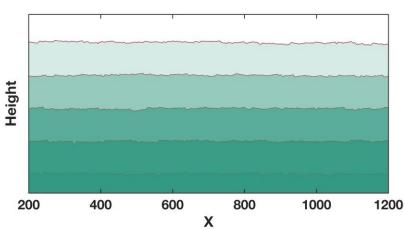
"Universality of dissipative self-assembly from quantum dots to human cells," Ilday, et al., Nature Physics, 2020



# Simply complex Lab



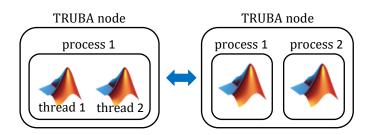


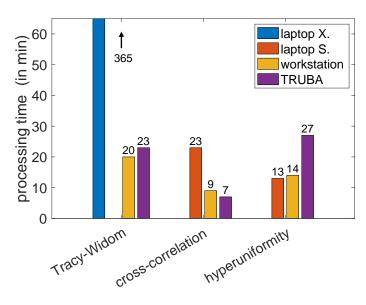


#### Code parallelization

#### MATLAB on TRUBA

- license requirements
- job queue
- auto-copy of figures, data, etc.
- very few code adjustments
- try optimize nr of threads!

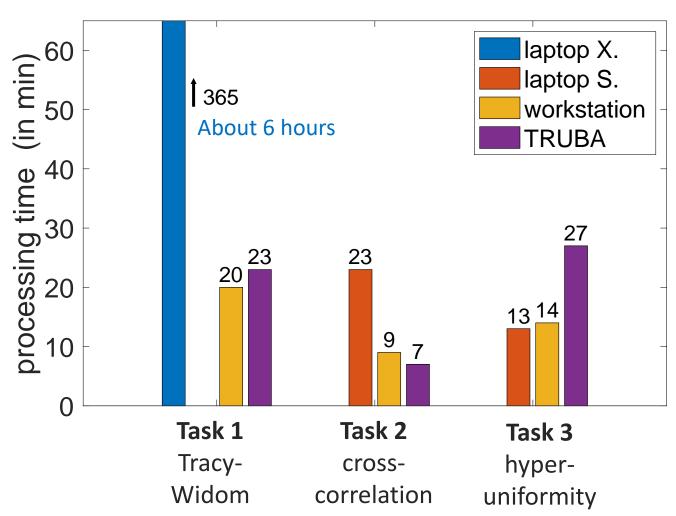




_	machine	cores	RAM	Resources
	laptop X.	2	16 GB	single-user
	laptop S.	8	32 GB	single-user
١	workstation	32	128 GB	multi-user
T	RUBA node	28	±100 GB	job queue







machine	cores	RAM	Resources
laptop X.	2	16 GB	single-user
laptop S.	8	32 GB	single-user
workstation	32	128 GB	multi-user
TRUBA node	28	±100 GB	job queue

same nr. of workers

26 workers : 13 x 2 threads + 1

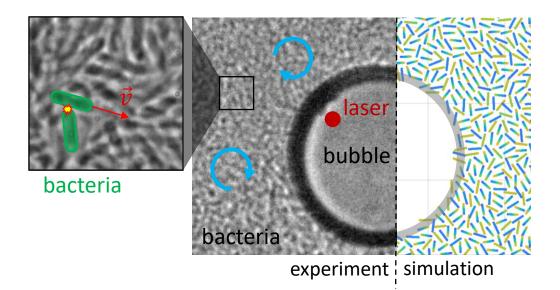
80% visualization → no speed-up

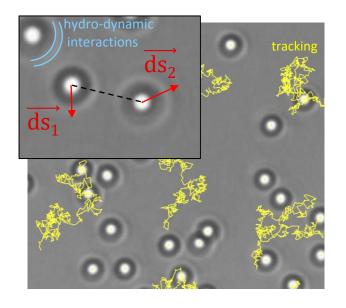


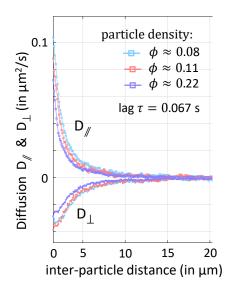
# Simply complex. Lab

#### Currently testing codes on TRUBA

- 1. Laser-material interaction (surface patterning)
- Other forms of universality (hyperuniformity)
- 3. Analysis of high frame-rate microscopy videos.
- 4. Bacterial turbulence simulations







#### Possible future usage TRUBA

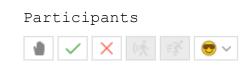
- 1. Colloidal particle diffusion & velocity correlation
- 2. Ultrafast laser oscillator simulations.
- 3. Laser-material interaction (ablation and heating).
- 4. Fluid dynamics.

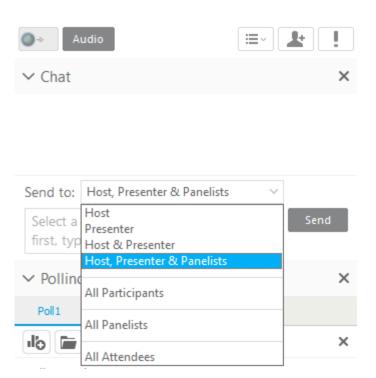
# Thank you



# Chatting

- Send to at least the Host,
   Presenter & Panelists
- Ideally, send to All Attendees







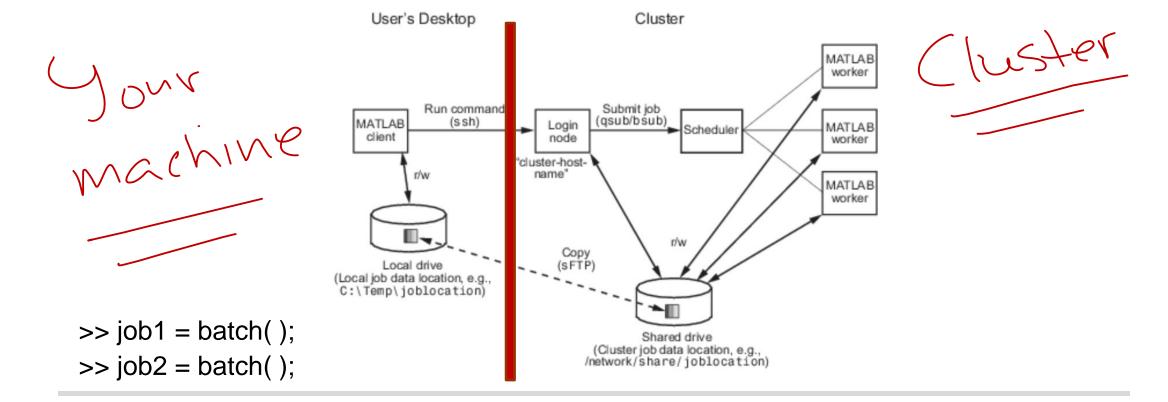
# A few notes about today's workshop

- The workflow and examples are about process, not performance
- MATLAB User Guide
  - https://docs.truba.gov.tr/how-to-guides/MATLAB/MATLAB\_TRUBA.html
- Requirements
  - MATLAB & Parallel Computing Toolbox R2021b
  - Account on TRUBA





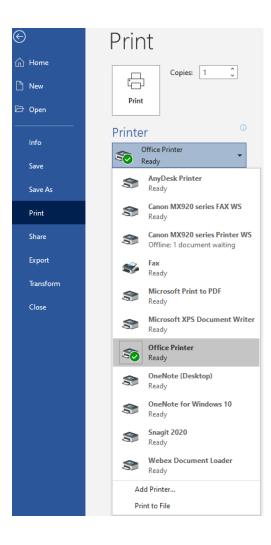
# Scaling MATLAB to TRUBA

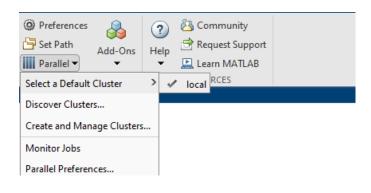


#SLURM ...
module load matlab
matlab ...



#### **Profiles**





"How does MATLAB know about TRUBA?"



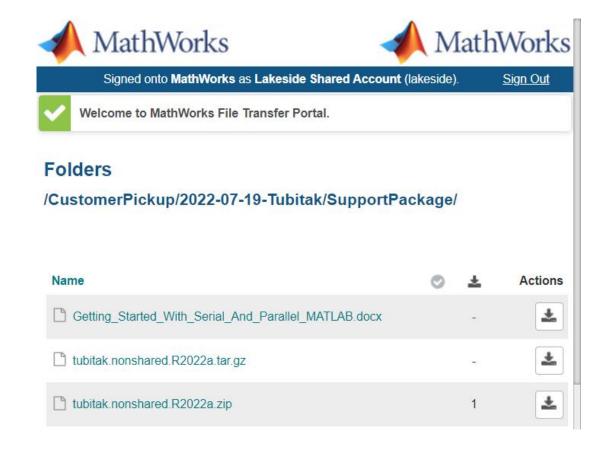


# Download the TRUBA MATLAB support package

#### https://tinyurl.com/Tubitak-Support-Package

- Username: Lakeside
- Password: 1qi6r47f
  - good until September 1, 2022
  - Will eventually be posted on TRUBA site

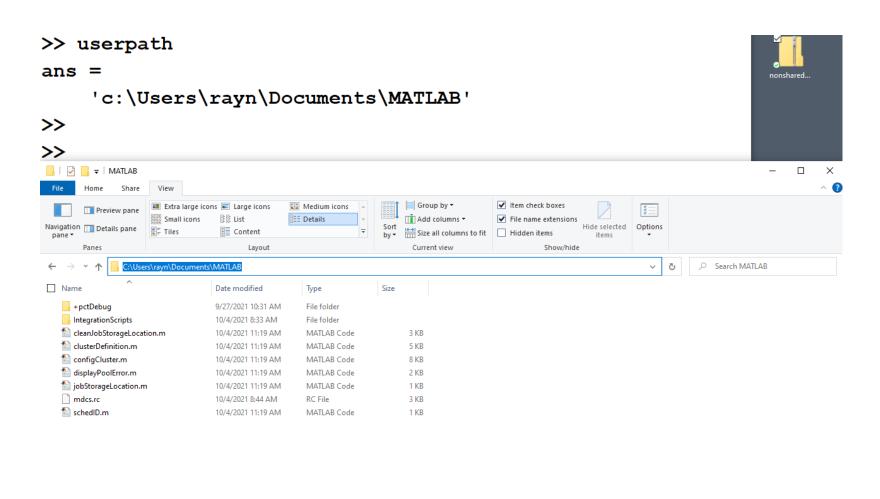
- Provides job hooks for
  - □ submission (**sbatch**)
  - □ state (**squeue**)
  - ☐ deletion (scancel)





# Install the support package – Windows

0 items





# Install the support package – Linux/macOS

```
[user@localhost ~] mkdir ~/Documents/MATLAB
[user@localhost ~] tar xf ~/tubitak.nonshared.R2022a.tar.qz -C ~/Documents/MATLAB
[user@localhost ~]
[user@localhost ~] ls -1 ~/Documents/MATLAB
+pctDebug
IntegrationScripts
cleanJobStorageLocation.m
clusterDefinition.m
clusterQueues.m
configCluster.m
displayPoolError.m
fixConnection.m
jobStorageLocation.m
mdcs.rc
schedID.m
```



## Configure MATLAB to create TRUBA profile

```
Set to your
                                                 user-id
>> configCluster
Username on TRUBA (e.g. joe): my-user-id
Complete. Default cluster profile set to "truba R2021b".
    Must set WallTime before submitting jobs to TRUBA. E.g.
    >> c = parcluster;
    >> % 5 hours
    >> c.AdditionalProperties.WallTime = '05:00:00';
    >> c.saveProfile
```

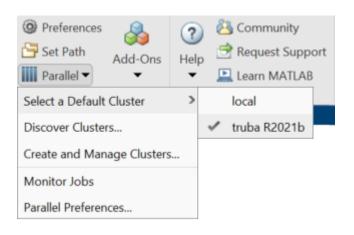


#### WORKSHOP-ONLY: Add reservation

```
>> % Add reservation for today's workshop
>> c.AdditionalProperties.Reservation = 'matlab';
>> c.saveProfile
```



# New TRUBA profile







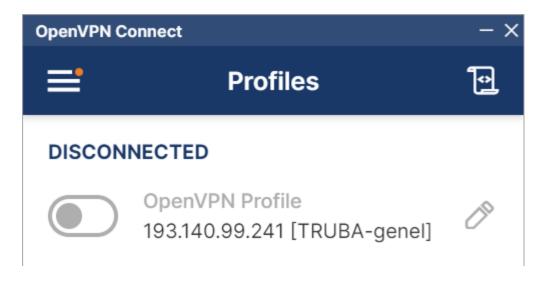
# MATLAB job submitters

- parpool
  - Single session
  - Synchronous execution
  - Seamlessly runs parfor, parfeval, and spmd

- batch
  - Multiple submissions
  - Non-blocking
  - Calls top-level function or script
  - Requires API to extract results



# VPN Connection – Required if not on ULAKNET





#### Exercise: "Hello, World!"

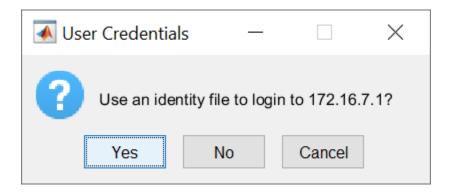
```
>> % Submit job to cluster to find out where MATLAB is running
>> % Get handle to HPC cluster
>> c = parcluster;
>> job = c.batch(@pwd,1,{}, 'CurrentFolder','.');

#SBATCH...
module load matlab
```

matlab ...



# SSH credentials (private key/passphrase or password)







## Fetching results

```
>> % Submit job to cluster to find out where MATLAB is running
>> % Get handle to HPC cluster
>> c = parcluster;
>> job = c.batch(@pwd,1,{}, 'CurrentFolder','.');
additionalSubmitArgs =
    '--ntasks=1 -N 1 -c 28 --ntasks-per-core=1 -t 00:10:00 -p hamsi'
>>
>> % Check the state of the job
>> job.State
ans =
    'finished'
>>
>> % Fetch the results
>> job.fetchOutputs{:}
ans =
    '/truba/home/rnorris'
```



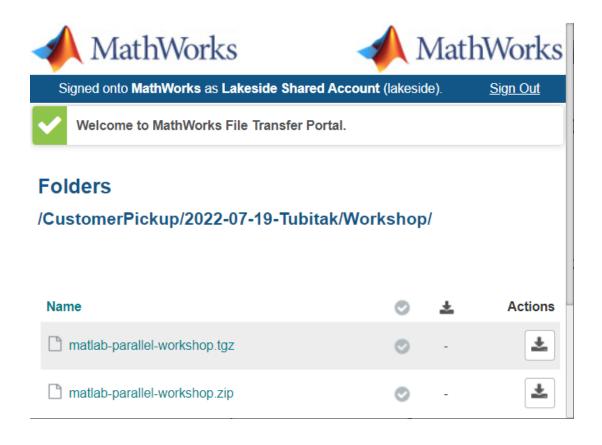
# Benign warning if CurrentFolder isn't set

```
>> job.fetchOutputs{:}
Warning: The task with ID 1 issued the following warnings:
    Warning: Worker unable to change folder to 'C:\Users' at the start of the batch
    job. The job will be executed from '/truba/home/rnorris'. To execute from a
    different folder use the 'CurrentFolder' parameter of batch. To suppress this
    warning, set 'CurrentFolder' to '.'.
```



## Download the workshop files

https://tinyurl.com/Tubitak-Workshop

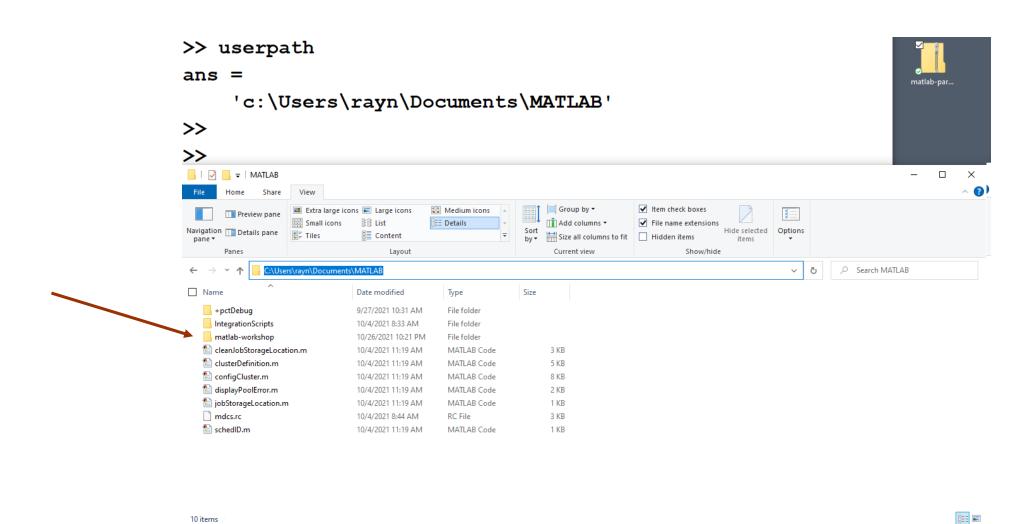


```
calc fft cpu gpu.m
calc mandelbrot.m
calc pi.m
mandelbrot example.m
parallel example.m
process files v1.m
process files v2.m
solve sys linear eqns.m
test fcn.m
```



# Install workshop files – Windows

10 items



29



# Install workshop files – Linux/macOS

```
[user@localhost ~] # mkdir -p ~/Documents/MATLAB
[user@localhost ~] # tar xf ~/matlab-parallel-workshop.tgz -C ~/Documents/MATLAB
[user@localhost ~]#
[user@localhost ~] # ls -1 ~/Documents/MATLAB/matlab-workshop
calc_fft_cpu_gpu.m
calc mandelbrot.m
calc_pi.m
mandelbrot_example.m
parallel_example.m
process_files_v1.m
process_files_v2.m
solve_sys_linear_eqns.m
test_fcn.m
```



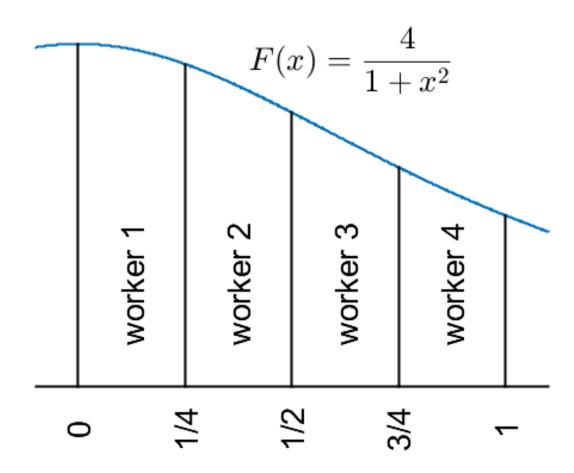
# Change directories to workshop

>> cd(fullfile(userpath, 'matlab-workshop'))



#### Exercise: Calculate $\pi$

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





#### Calculate $\pi$

```
function calc pi
spmd
    a = (labindex - 1) / numlabs;
    b = labindex/numlabs;
    fprintf('Subinterval: [\$-4g, \$-4g] \setminus n', a, b)
    myIntegral = integral(@quadpi, a, b);
    fprintf('Subinterval: [%-4g, %-4g] Integral: %4g\n', a, b, myIntegral)
   piApprox = gplus(myIntegral);
end
approx1 = piApprox{1}; % 1st element holds value on worker 1
fprintf('pi
                    : %.18f\n', pi)
fprintf('Approximation: %.18f\n', approx1)
fprintf('Error : %g\n', abs(pi - approx1))
function y = quadpi(x)
%QUADPI Return data to approximate pi.
% Derivative of 4*atan(x)
y = 4./(1 + x.^2);
```



# Where should you start a local parallel pool?

```
function parallel_example

parp(ol(4);

parfor idx = 1:8
    A(idx) = rand;
end
```

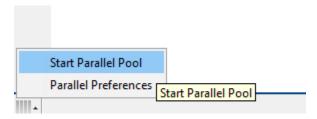
"What will happen the next time you run this code?"

Error using <u>parpool</u>
Found an interactive session. You cannot have multiple interactive sessions open simultaneously.



# How should you start a local parallel pool?

- Call parpool from the Command Window
- Have MATLAB automatically start a parallel pool if it hasn't already started
- From the lower lefthand corner





# Then how do I tell the cluster my job needs a parallel pool?

```
job = c.batch(.., 'Pool',pool_size);
```



# Submit calc pi job

```
>> % Submit calc_pi job
>> c = parcluster;
>>
>> % Request 3 workers
>> job = c.batch(@calc_pi,0,{}, 'CurrentFolder','.', 'Pool',3);
additionalSubmitArgs =
    '--ntasks=4 -N 1 -c 7 --ntasks-per-core=1 -t 00:10:00 -p hamsi'
?
```

"If my Pool is size 3, why am I requesting 4 tasks?"



### "The Power of 28"

- hamsi partition
  - dual socket nodes, with 28 cores per socket
  - Multiples of 28 cores need to be consumed by your job



- Therefore, the total number of workers must either be
  - a factor of 28 (1, 2, 4, 7, or 14) or
  - a multiple of 28 (28, 56, 84, 112, etc.)



## Requesting <= 28 workers

- Request a pool of **0**,**1**,**3**,**6**,**13**, or **27** workers
  - If NumThreads is 1 (default), we'll adjust the thread count to fit on a single node

```
>> job = c.batch(@pwd,1,{}, 'CurrentFolder','.', 'Pool', 3);
additionalSubmitArgs =
    '--ntasks=4 -N 1 -c 7 --ntasks-per-core=1 -t 00:10:00 -p hamsi'
>>
>>
>> job = c.batch(@pwd,1,{}, 'CurrentFolder','.', 'Pool', 2);
Error using <u>parallel.Cluster/batch</u> (<u>line 158</u>)
Job submission failed because the plugin function
'communicatingSubmitFcn.m' errored.
Caused by:
   Error using getCommonSubmitArgs (line 37)
```

Error 1: ProcsPerNode (28) must be evenly divisible by NumWorkers (3)



## Requesting > 28 workers

Request multiples of 28 workers

```
>> job = c.batch(@pwd,1,{}, 'CurrentFolder','.', 'Pool', 55);
additionalSubmitArgs =
    '--ntasks=56 -N 2 -c 1 --ntasks-per-core=1 -t 00:10:00 -p hamsi'
>>
>>
>> job = c.batch(@pwd,1,{}, 'CurrentFolder','.', 'Pool', 30);
Error using <u>parallel.Cluster/batch</u> (<u>line 158</u>)
Job submission failed because the plugin function
'communicatingSubmitFcn.m' errored.
Caused by:
   Error using getCommonSubmitArgs (line 42)
    Error 2: NumWorkers (31) * NumThreads (1) must be evenly divisible by
```



### Fetch the results

```
>> % Submit calc pi job
>> c = parcluster;
>>
>> % Request 3 workers
>> job = c.batch(@calc_pi(0){}, 'CurrentFolder','.', 'Pool',3);
additionalSubmitArgs =
    '--ntasks=4 -N 1 -c 7 --ntasks-per-core=1 -t 00:10:00 -p hamsi'
>>
                                                            "Where's the
>> % Check the state of the job
                                                           output?"
>> job.State
ans =
    'finished'
>>
>> % Fetch the results
>> job.fetchOutputs{:}
>>
```



# What gets "returned"?

- Function output
- Diary
- Saved files



### Example

```
function [t, A] = test fcn(sims)
disp('Start sim')
t0 = tic;
parfor idx = 1:sims
    A(idx) = idx;
    pause (0.5)
    idx
end
t = toc(t0);
disp('Finished')
save RESULTS A
```



### Job submission

```
>> job = c.batch(@test_fcn,1,{300}, 'CurrentFolder','.', 'Pool',6);
additionalSubmitArgs =
   '--ntasks=7 -N 1 -c 4 --ntasks-per-core=1 -t 00:10:00 -p hamsi'
```



### Fetch output

```
function [t, A] = test_fcn(sims)
c.batch(@test_fcn(1){300},
```





# Diary

```
>> % View the diary
>> job.diary
--- Start Diary ---
Start sim
ans =
     4
ans =
     5
ans =
     8
```

```
function [t, A] = test_fcn(sims)
disp('Start sim')

t0 = tic;
parfor idx = 1:sims
    A(idx) = idx;
    pause(0.5)
    idx
end
t = toc(t0);
disp('Finished')
save RESULTS A
```



### Save files

```
function [t, A] = test fcn(sims)
                   disp('Start sim')
"Where does RESULTS
   get written to?"
                   t0 = tic;
                   parfor idx = 1:sims
                     A(idx) = idx;
                     pause (0.5)
                     idx
                   end
                   t = toc(t0);
                   disp('Finished')
                   save RESULTS A
```



### Other settable job properties (1)

```
>> c.AdditionalProperties
ans =
 Additional Properties with properties:
                 AccountName: ''
        AdditionalSubmitArgs: ''
                 ClusterHost: '172.16.7.1'
                EmailAddress: ''
                 EnableDebug: 0
                ProcsPerNode: 28.00
                   QueueName: 'hamsi'
   RemoteJobStorageLocation:
        RequireExclusiveNode: 0
                 Reservation: ''
             UseIdentityFile: 0
                     UseSmpd: 0
                    Username:
                    WallTime: '00:10:00'
```



# Other settable job properties (2)

- AccountName
- EmailAddress
- Reservation
- WallTime



### Submitting scripts, instead of functions

```
>> x = 4;
\gg z = rand(3);
>>
>> % Submit a script (instead of a function)
>> job = c.batch('temp = rand(10); y = x, who', 'CurrentFolder','.');
additionalSubmitArgs =
    '--ntasks=1 -N 1 -c 28 --ntasks-per-core=1 -t 00:10:00 -p hamsi'
>> clear z
>>
>> who
Your variables are:
    job x
C
>> % Check the state of the job
>> job.State
ans =
    'finished'
```



### Loading variables to local workspace

>> % Load variables
>> job.load
>> who

"If we cleared z, then why does who display it?

And I didn't need temp!



Your variables are:

ans c job temp x y

>> job.diary
--- Start Diary ---

**y** =

4

Your variables are:



--- End Diary ---

"I'll pass all the variables in your local workspace to all of the workers. Then I'll pass everything the workers generate and pass it back to your local workspace."

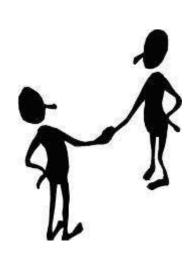




## Adding files to the job

### AdditionalPaths

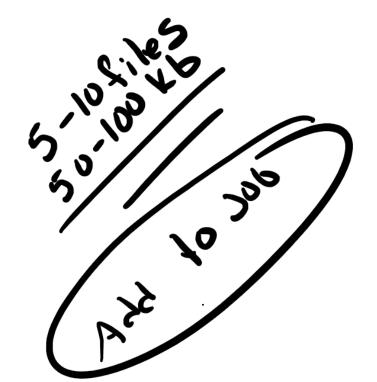
- List absolute paths on the cluster (include subdirectories if needed)
- AttachedFiles
  - List files not automatically added to the job (e.g., binary files)
- AutoAddClientPath
  - Set to false if you have added your own local paths to the MATLAB client path
- AutoAttachFiles
  - Useful for small number, often changing files

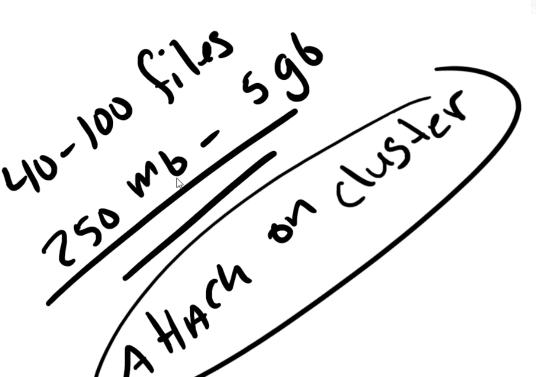


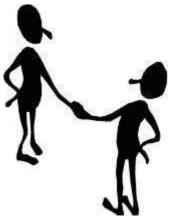


## Should I send files with the job?

- By default, each job will copy all required files
  - How many jobs are you going to submit?
  - How large, in totality, are your files?
  - Do your files change a lot?









## When has my job run and finished?

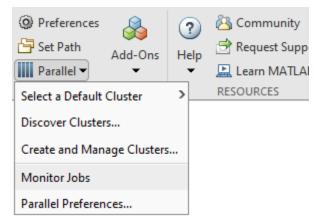
To be used sparingly, ... (can have impact on network)

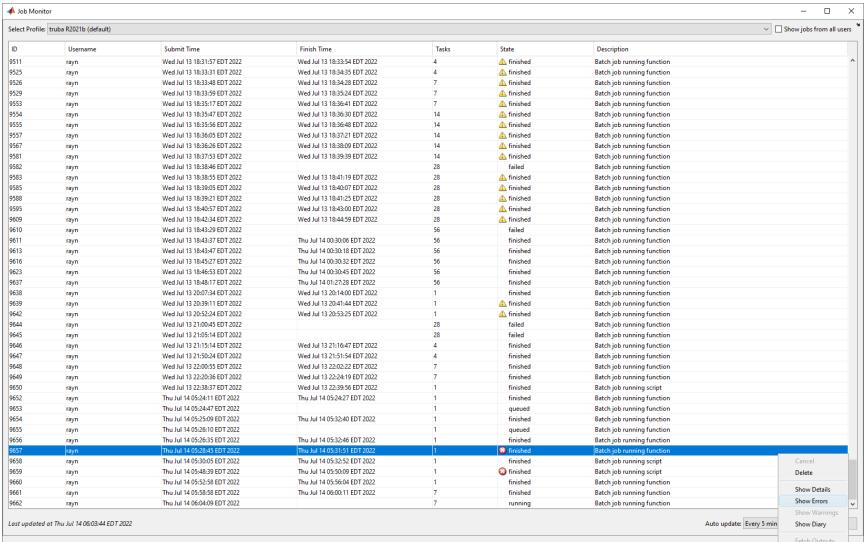


```
>> % Get email notification when my job has finished running
>> c.AdditionalProperties.EmailAddress = 'user-id@tubitak.gov.tr';
>> job = c.batch(@test_fcn,1,{300}, 'CurrentFolder','.', 'Pool',6);
additionalSubmitArgs =
   '--ntasks=7 -N 1 -c 4 --ntasks-per-core=1 -t 00:10:00 -p hamsi --mail-type=ALL
```



## Retrieving past jobs







### Keep cluster clean: delete jobs

As a good practice, delete jobs you no longer need anymore

```
>> % Finished with the job, delete it to cleanup jobs
>> job.delete
```



# Debugging and Troubleshooting





### Scheduler ID

```
>> job = c.batch(@pwd,1,{}, 'CurrentFolder','.');
additionalSubmitArgs =
    '--ntasks=1 -N 1 -c 28 --ntasks-per-core=1 -t 00:10:00 -p hamsi'
>>
>> % Job ID vs Scheduler ID
>> job.ID
ans =
        9656
>>
>> job.getTaskSchedulerIDs{1}
ans =
    '208426'
```



### Example: Errored jobs

```
>> % Undefined function
>> job = c.batch(@invalid_fcn,1,{}, 'CurrentFolder','.');
additionalSubmitArgs =
    '--ntasks=1 -N 1 -c 28 --ntasks-per-core=1 -t 00:10:00 -p hamsi'
>>
>> % Undefined variable in a script
>> job2 = c.batch('x = y', 'CurrentFolder','.');
additionalSubmitArgs =
    '--ntasks=1 -N 1 -c 28 --ntasks-per-core=1 -t 00:10:00 -p hamsi'
```



### Errored jobs (1)

```
>> % Undefined function
>> job.State
ans =
    'finished'
>>
>> job.fetchOutputs{:}
Error using parallel.Job/fetchOutputs (line 1300)
An error occurred during execution of Task with ID 1.
Caused by:
    Unrecognized function or variable 'invalid fcn'.
```



## Errored jobs (2)

```
>> % Undefined variable in a script
>> job2.load
Error using parallel.Job/load (line 36)
Error encountered while running the batch job. The error was:
Unrecognized function or variable 'y'.

If 'y' is a file that is required by 'x = y', add the full path name for 'y' to the batch job's AttachedFiles property. For more information, see batch.
```



### Logfile: Single core job

```
>> job = c.batch(@test_fcn,1,{300}, 'CurrentFolder','.');
additionalSubmitArgs =
    '--ntasks=1 -N 1 -c 28 --ntasks-per-core=1 -t 00:10:00 -p hamsi'
>>
>> % Retrieve log file for single core job
>> c.getDebugLog(job.Tasks)
LOG FILE OUTPUT:
Executing: /truba/sw/centos7.9/app/matlab/r2021b/bin/worker
Exiting with code: 0
```



### Logfile: Multi-core job

```
>> job = c.batch(@test_fcn,1,{297}, 'CurrentFolder','.', 'Pool',27);
additionalSubmitArgs =
    '--ntasks=28 -N 1 -c 1 --ntasks-per-core=1 -t 00:10:00 -p hamsi'
>>
    % Retrieve log file for multi-core job
>> c.getDebugLog(job)
LOG FILE OUTPUT:
The scheduler has allocated the following nodes to this job:
hamsi37
"/truba/sw/centos7.9/app/matlab/r2021b/bin/mw_mpiexec" -bind-to core -l -n 28 "/truba
[0] Sending a stop signal to all the labs...
[0] Parallel pool is shutting down.[0]
Exiting with code: 0
```



### WORKSHOP-ONLY: Remove reservation

```
>> % Remove reservation from future jobs
>> c.AdditionalProperties.Reservation = '';
>> c.saveProfile
```



### From Coding to Cluster (1)

```
% Notes - From Coding to Cluster
% 1. Using a script, not a function
% 2. Paths are hardcoded
% 3. File separator is hard coded
% 4. Assumes TIF file exists
% 5. TIF files must be on the MATLAB path
% 6. Assumes output folder already exists where ever MATLAB is running
% 7. Results MAT-File will be overwritten next time it's run
% 8. Changes MATLAB working directory
filelist = dir('tif\*.tif');
fileNames = {filelist.name}';
segmentedCellSequence = batchProcessFiles(@detectCells,fileNames);
cd output
save SCS segmentedCellSequence
```



```
function [ofile, segmentedCellSequence] = process files v2(rootd,outd)
if nargin==0
    rootd = fullfile(pwd, 'tif');
    outd = fullfile(pwd, 'output');
end
filelist = dir(fullfile(rootd, '*.tif'));
if isempty(filelist)
    error('Failed to find image files: %s',rootd)
end
fileNames = {filelist.name}';
addpath (rootd)
segmentedCellSequence = batchProcessFiles(@detectCells,fileNames);
% Ensure output directory exists
if exist(outd,'dir')==false
    [FAILED, emsg, eid] = mkdir(outd);
    if FAILED==true
        error(eid,emsg)
    end
end
% Add timestamp for file uniqueness
ts = strrep(strrep(datestr(now), ' ', '_'), ':', '-');
% Save dir
old dir = pwd;
c = onCleanup(@()cd(old dir));
cd (outd)
ofile = ['SCS ' ts];
save(ofile,'segmentedCellSequence')
```



### Run it locally

```
>> % Start local parallel pool
>> parpool(4);
Starting parallel pool (parpool) using the 'local' profile ...
Connected to the parallel pool (number of workers: 4).
>>
>> % Call the function locally
>> ofile = process files v2
ofile =
    'S:\sandbox\Workshops\Parallel-Computing-Workshop\matlab-workshop-files'
>>
```



### Run it on the cluster

```
>> % Submit job to cluster
>> c = parcluster;
>> j = c.batch(@process_files_v2, 1, {'/work/raymond/proj-tiffs','/home/raymond/output-results'},'Pool',3);
>> % Wait for job to finish
>> j.wait
>>
>> % Fetch the results
>> ofile = j.fetchOutputs{:}

ofile =
    '/home/raymond/output-results/SCS_27-Apr-2021_16-54-28'
>>
```



## From Coding to Cluster (2)

```
% Notes - From Coding to Cluster
% 1. Using a script, not a function
        return status or output directory
% 2. Paths are hardcoded
       pass in root directory
% 3. File separator is hard coded
       use fullfile
% 4. Assumes TIF file exists
        check results when touching the file system
% 5. TIF files must be on the MATLAB path
        add tif folder to the MATLAB path
 6. Assumes output folder already exists where ever MATLAB is running
        supply output directory to write to. check if folder exists; if
       not, create it
 7. Results MAT-File will be overwritten next time it's run
        add timestamp to filename
% 8. Changes MATLAB working directory
        Track old directory, change back before leaving
```

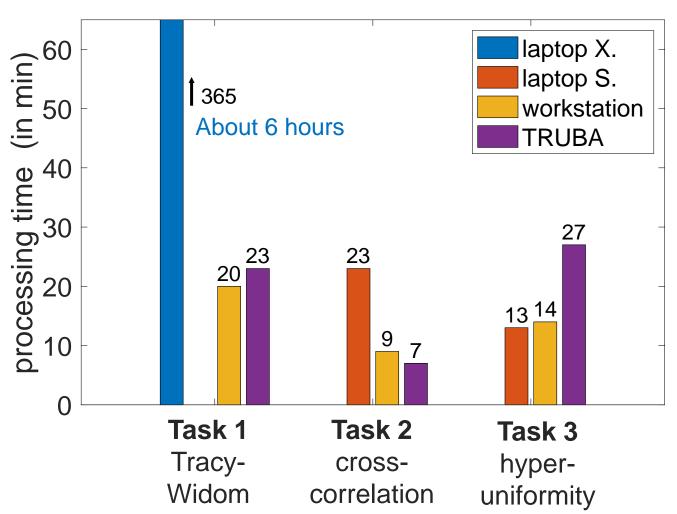


### Running bulk jobs

```
function jobs = submit jobs
c = parcluster;
c.AdditionalProperties.EmailAddress = 'my-email@work';
sims = [54 \ 162 \ 324 \ 648];
for sidx = 1:length(sims)
    % Run code with different number of iterations
    jobs(sidx) = c.batch(@parallel_example,1,{sims(sidx)}, 'Pool',3);
end
% Wait for the 2nd job to finish
jobs (2) .wait
t = jobs(2).fetchOutputs{:}
```







	machine	core s	RAM	Resources
	laptop X.	2	16 GB	single-user
	laptop S.	8	32 GB	single-user
	workstation	32	128 GB	multi-user
	TRUBA node	28	±100 GB	job queue

same nr. of workers

26 workers: 13 x 2 threads + 1

80% visualization→ no speed-up



### Workstation or TRUBA?

### Workstation

- Plusses
  - "Immediate" access
  - Easier MATLAB licensing
- Deltas
  - Cost and procurement of each workstation
  - Waste when it's not being used
  - 1 job at a time

### TRUBA

- Plusses
  - An abundant of compute resources
  - Able to run a collection of jobs at once
- Deltas
  - Each node is a bit less powerful than a workstation
  - Need to configure MATLAB licensing
  - Transferring files/data to TRUBA



### How do I get started?

- Need to point MATLAB Parallel Server to your own university license
- Contact
  - Sefa Arslan
  - sefa.arslan@tubitak.gov.tr

"How do I license MATLAB Parallel Server?"





## Summary – Remote Submission

- Call configCluster (once) to create TRUBA profile
- Toggle between local profile (desktop machine) and TRUBA profile (multinode)
- Tuning your job with AdditionalProperties
- Best practices for job submission and troubleshooting
- Contact Tubitak to get started