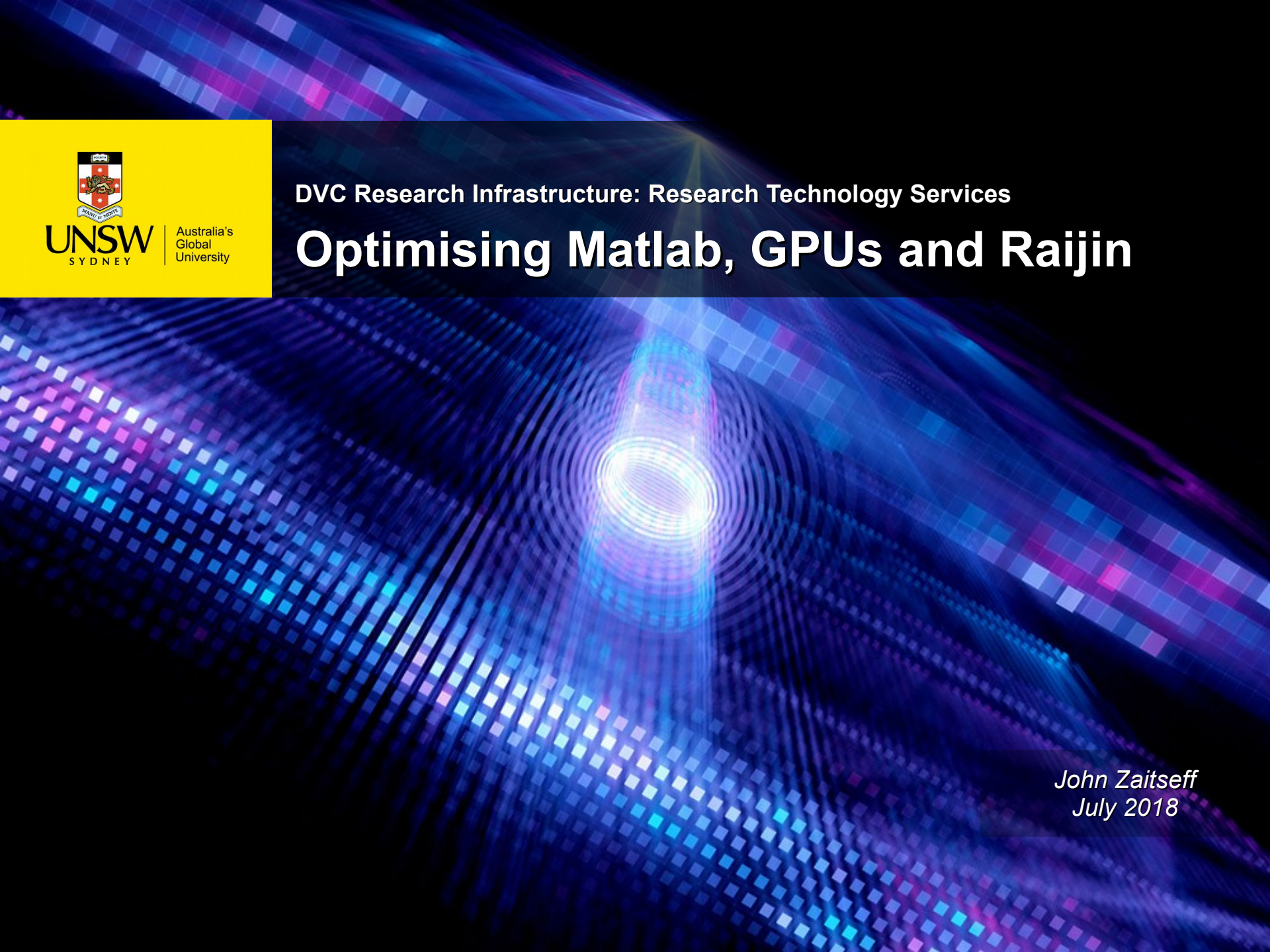

DVC Research Infrastructure: Research Technology Services

Optimising Matlab, GPUs and Raijin

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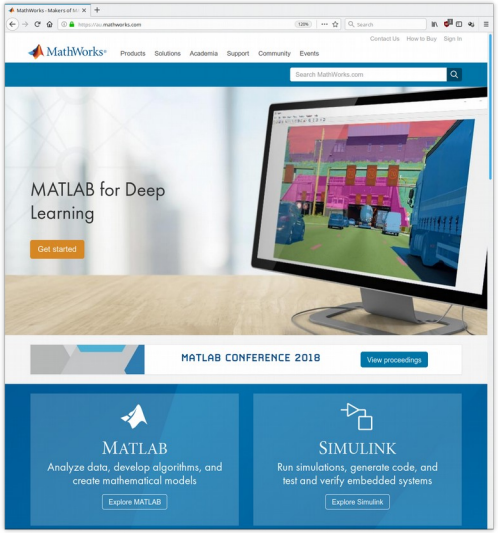
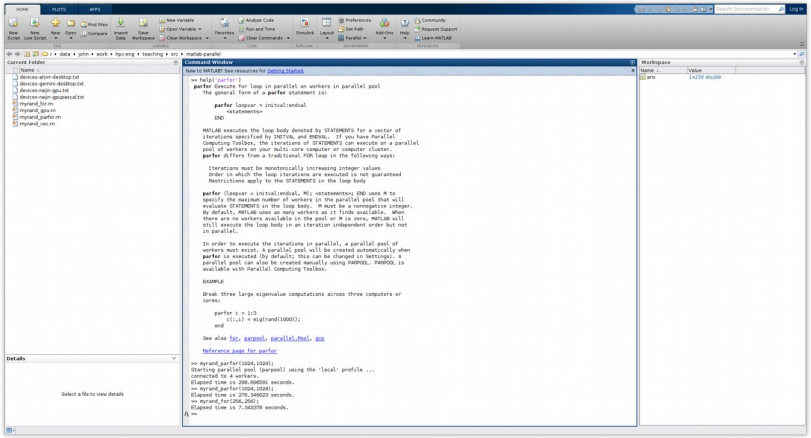
Optimising your Matlab code

1. Register an account on the Mathworks website
   - *https://www.mathworks.com/*
   - Free access to documentation, instructional videos, examples, benchmarks and discussion groups
2. Read the Matlab documentation
   - Particularly **Support » Documentation » Parallel Computing Toolbox » Getting Started**
3. Profile your code
4. Check your algorithms
5. Vectorise your code
6. Use GPUs with `gpuArray`
7. Use `parfor`, `parfeval` and `spmd`
8. Talk to others!



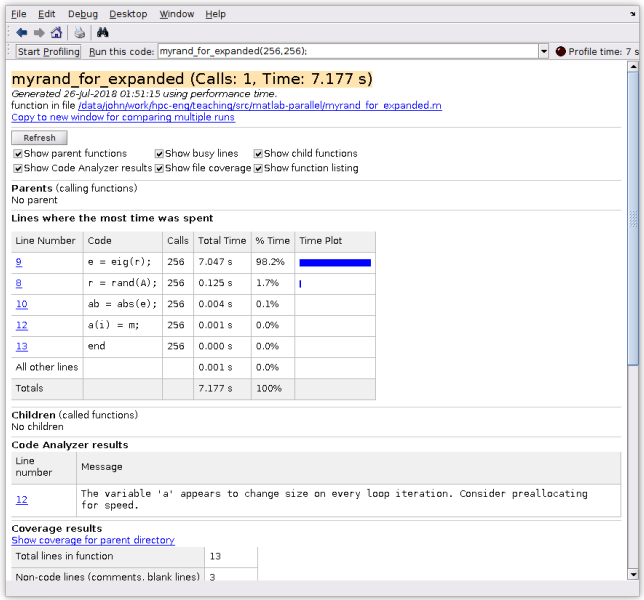


Profile your code

"The real problem is that programmers have spent far too much time worrying about efficiency in the wrong places and at the wrong times; **premature optimisation is the root of all evil** (or at least most of it) in programming."

> — Donald Knuth, "Computer Programming as an Art", *Communications of the ACM* **17** (12), December 1974, p. 671, emphasis added.

- Where is your code spending its time?
- Use Matlab's built-in tools
  - `profile viewer` for a graphical interface
  - `tic` and `toc` for basic timing
  - `mpiprofile` for parallel code
- Focus on areas consuming the majority of time
- Evaluate the effectiveness of your algorithms
- Use built-in functions and toolboxes where possible
  - "Built-in Parallel Computing Support" help topic



Vectorise your code

- Where possible, convert your code from `for` loops to matrix and vector operations
  - Code looks more like mathematical expressions
  - Code is often shorter
  - Code often runs significantly faster
  - Often a prerequisite for good GPU performance
- Example using vectors:

```
i = 0;
for t = 0 : 0.01 : 10
    i = i + 1;
    y(i) = sin(t);
end
```

```
t = 0 : 0.01 : 10;
y = sin(t);
```

- Example using arrays:

```
for n = 1 : 10000
   V(n) = 1/12 * pi * (D(n) ^ 2) * H(n));
end
```

```
V = 1/12 * pi * (D .^ 2) .* H;
```

Use `parfor`, `parfeval` and friends

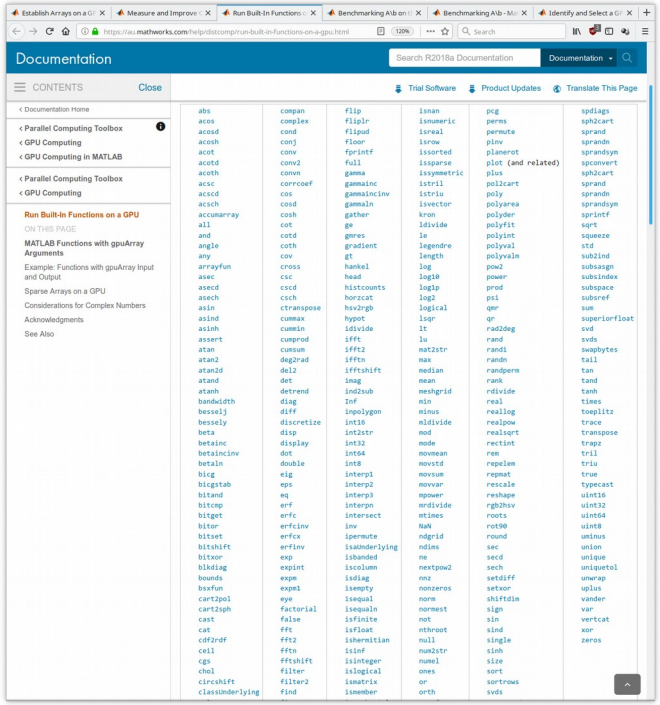
- Examine your code for time-consuming `for` loops and replace with `parfor`
  - Each iteration must be *independent* (must not depend on the results) of other iterations
  - Reduction variables (e.g., loop summation) are allowed
  - Converting outer `for` loops work best
  - e.g., Monte Carlo simulations
  - e.g., Parameter sweeps
- Other possibilities: `parfeval`, `distributed`, `datastore`, `mapreduce`, `spmd`
- Can use all cores of a multiprocessor compute node
  - On Raijin: **normal** queue – up to 16 cores; **normalbw** queue – up to 28 cores
- Example:

```
for i = 1 : N
  a(i) = max(abs(eig(rand(A))));
end
```

```
parfor i = 1 : N
  a(i) = max(abs(eig(rand(A))));
end
```

Use GPUs with `gpuArray`

- Read the “GPU Computing in Matlab” help topic
- Check GPU device capabilities with `gpuDevice`
- Use `gpuArray` to create arrays on or copy arrays to the GPU
- Use `gather` to copy arrays back from the GPU
- Check which inbuilt functions can run on the GPU
  - “Run Built-In Functions on a GPU” help topic
  - Currently 344 intrinsic functions
- Profile using `tic`, `toc`, `gputimeit`
- Consider using single-precision calculations
- Example:




```
r_cpu = rand(1024);
r_gpu = rand(1024, 'gpuArray');
m = eig(r_gpu);
isOnGPU(m)
```

% `r_cpu` array is on the CPU
% `r_gpu` array is on the GPU
% Do a calculation on the GPU
% `isOnGPU` returns 1 (true)

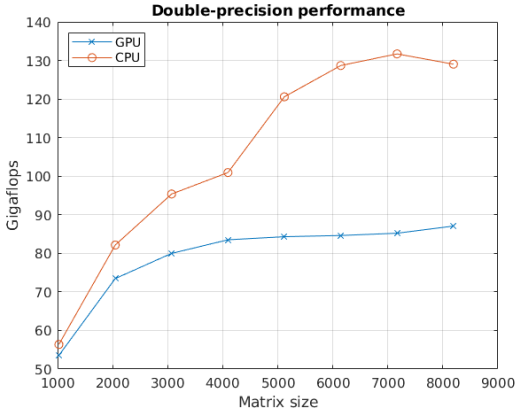
Using GPUs on Raijin

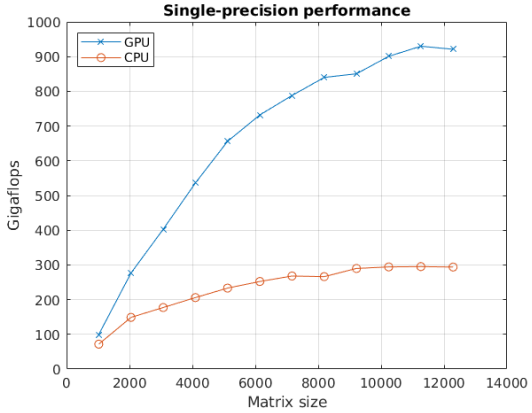
- Read the *GPU User Guide* at *https://opus.nci.org.au/display/Help/GPU+User+Guide*
- Raijin currently has
  - **gpu** queue:
    · 30 nodes of four Nvidia K80 accelerators (eight GPUs) each,
    · up to 2.91 teraFLOPS double-precision performance per GPU,
    · up to 8.73 teraFLOPS single-precision performance per GPU,
    · 18 SU (72¢ in-kind contribution) per hour per GPU
  - **gpupascal** queue:
    · 2 nodes of four Nvidia P100 GPUs each,
    · up to 5.3 teraFLOPS double-precision performance per GPU,
    · up to 10.6 teraFLOPS single-precision performance per GPU,
    · 24 SU (96¢ in-kind contribution) per hour per GPU
- Develop code on your workstation or desktop computer
  - Can also use Raijin interactively! Use "`ssh -Y`" or **MobaXterm** with inbuilt X server

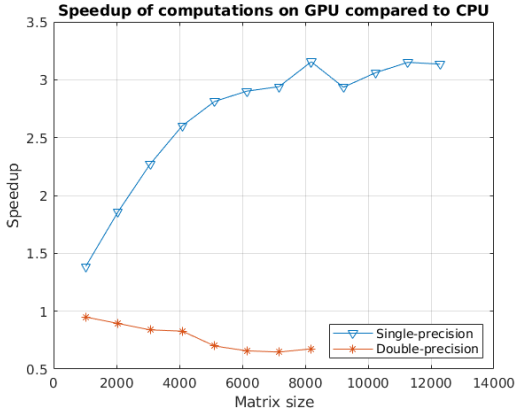
```
qsub -q gpu -l ngpus=2 -l ncpus=6 -l software=matlab_unsw \
     -l walltime=0:30:00 -l mem=32GB -I -X

module load matlab
matlab &
```

Why use Raijin? Scale, performance, cost

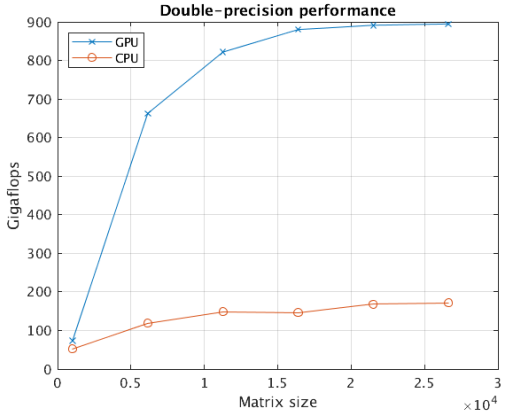
- Desktop computer with Nvidia GTX760: `paralleldemo_gpu_backslash(0.6)`

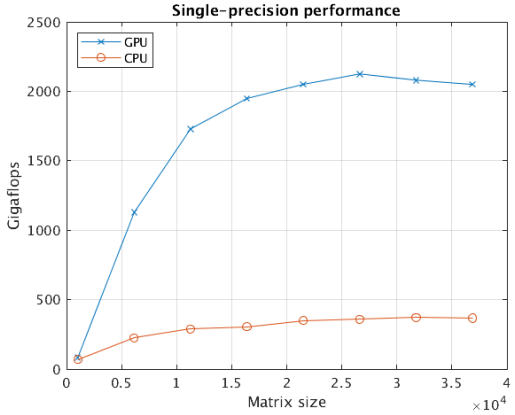


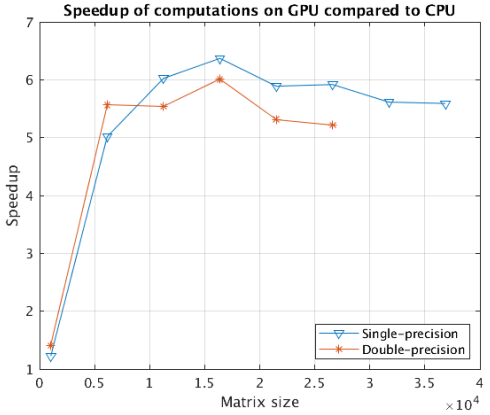




- Raijin K80 node (**gpu** queue), one GPU: `paralleldemo_gpu_backslash(6.0)`







Talk to us!

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