Parallel Computing with MATLAB

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Overview

- Scene setting
- Task Parallel (`par*`)
- Why doesn’t it speed up as much as I expected?
- Data parallel (`spmd`)
- GPUs

What I assume

- Reasonable MATLAB knowledge
  - e.g. vectorization, pre-allocation
- Some use of PCT and associated concepts
  - What is a cluster
  - Simple `parfor` usage

`parfor`

Definition

Code in a `parfor` loop is guaranteed by the programmer to be execution order independent

Why is that important?

We can execute the iterates of the loop in any order, potentially at the same time on many different workers.

A simple parfor loop

```
parfor i = 1:N
    out(i) = someFunction(in(i));
end
```

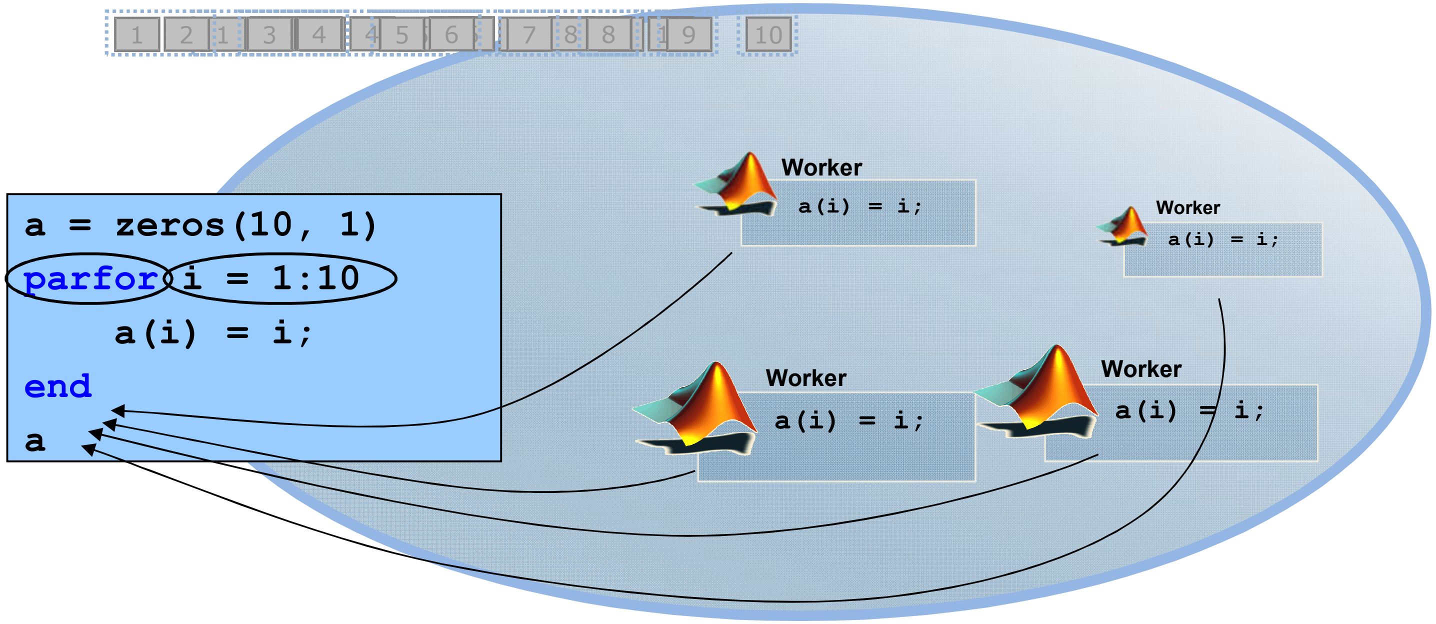
`parfor` – how it works

- A loop from 1:N has N *iterates* which we partition into a number of *intervals*
  - Each *interval* may have a different number of *iterates*

- Allocate the *intervals* to execute on the workers

- Stitch the results back together

The Mechanics of parfor Loops



parforIterateDemo

Pool of MATLAB Workers

Variable Classification

```
reduce = 0; bcast = …; in = …;
parfor i = 1:N
    temp = foo1(bcast, i);
    out(i) = foo2(in(i), temp);
    reduce = reduce + foo3(temp);
end
```

Loop variable

```
reduce = 0; bcast = …; in = …;
parfor i = 1:N
    temp = foo1(bcast, i);
    out(i) = foo2(in(i), temp);
    reduce = reduce + foo3(temp);
end
```

Making extra parallelism

- No one loop appears to have enough iterations to go parallel effectively

```
for ii = 1:smallNumber_I
    for jj = 1:smallNumber_J
        for kk = 1:smallNumber_K
        end
    end
end

smallNumber_I * smallNumber_J * smallNumber_K == quiteBigNumber
```

```
mergeLoopsDemo
```

Sliced Variable

```
reduce = 0; bcast = …; in = …;
parfor i = 1:N
    temp = foo1(bcast, i);
    out(i) = foo2(in(i), temp);
    reduce = reduce + foo3(temp);
end
```

Broadcast variable

```
reduce = 0; bcast = …; in = …;
parfor i = 1:N
    temp = foo1(bcast, i);
    out(i) = foo2(in(i), temp);
    reduce = reduce + foo3(temp);
end
```

Reusing data

```
D = makeSomeBigData;
converged = false;
while ~converged
    parfor jj = 1:M
        p(jj) = func(p, D);
    end
    [converged, result] = checkConverged(p)
end
```

Reusing data (new in 15b)

```
D = parallel.pool.Constant(@makeSomeBigData);
converged = false;
while ~converged
    parfor jj = 1:M
        p(jj) = func(p, D.value);
    end
    [converged, result] = checkConverged(p)
end
```

constantDemo

Counting events in parallel

- Inside the parallel loop you are looking to count the number of times some particular result is obtained
  - Histograms, interesting results, etc.

Reduction Variable

```
reduce = 0; bcast = …; in = …;
parfor i = 1:N
    temp = foo1(bcast, i);
    out(i) = foo2(in(i), temp);
    reduce = reduce + foo3(temp);
end
```

```
parforSearchDemo
```

Common parallel program

```
set stuff going
while not all finished {
    for next available result do something;
}
```

`parfeval`

- New feature in R2013b
- Introduces asynchronous programming

```
f = parfeval(@func, numOut, in1, in2, …)
```

- The return **`f`** is a future which allows you to
  - Wait for the completion of calling **`func(in1, in2, …)`**
  - Get the result of that call
  - … do other useful parallel programming tasks …

Fetch Next

- Fetch next available unread result from an array of futures.

```
[idx, out1, ...] = fetchNext(arrayOfFutures)
```

- **`idx`** is the index of the future from which the result is fetched
- Once a particular future has returned a result via **`fetchNext`** it will *never* do so again
  - That particular result is considered read, and will not be re-read

Common parallel program (MATLAB)

```
% Set stuff going
for ii = N:-1:1
    fs(ii) = parfeval(@stuff, 1);
end
% While not all finished
for ii = 1:N
    % for next available result
    [whichOne, result] = fetchNext(fs);
    doSomething(whichOne, result);
end
```

parfevalWaitbarDemo

Better parallel program

```
set N things going
while not all finished {
    set N more things going
    for N {
        for next available result do something;
    }
}
```

```
parfevalNeedleDemo
```

parfevalOnAll

- Frequently you want setup and teardown operations
  - which execute once on each worker in the pool, before and after the actual work
- Execution order guarantee:

It is guaranteed that relative order of `parfeval` and `parfevalOnAll` as executed on the client will be preserved on all the workers.

Why isn't it as fast as I expect?

- How fast did you expect?
  - Why?

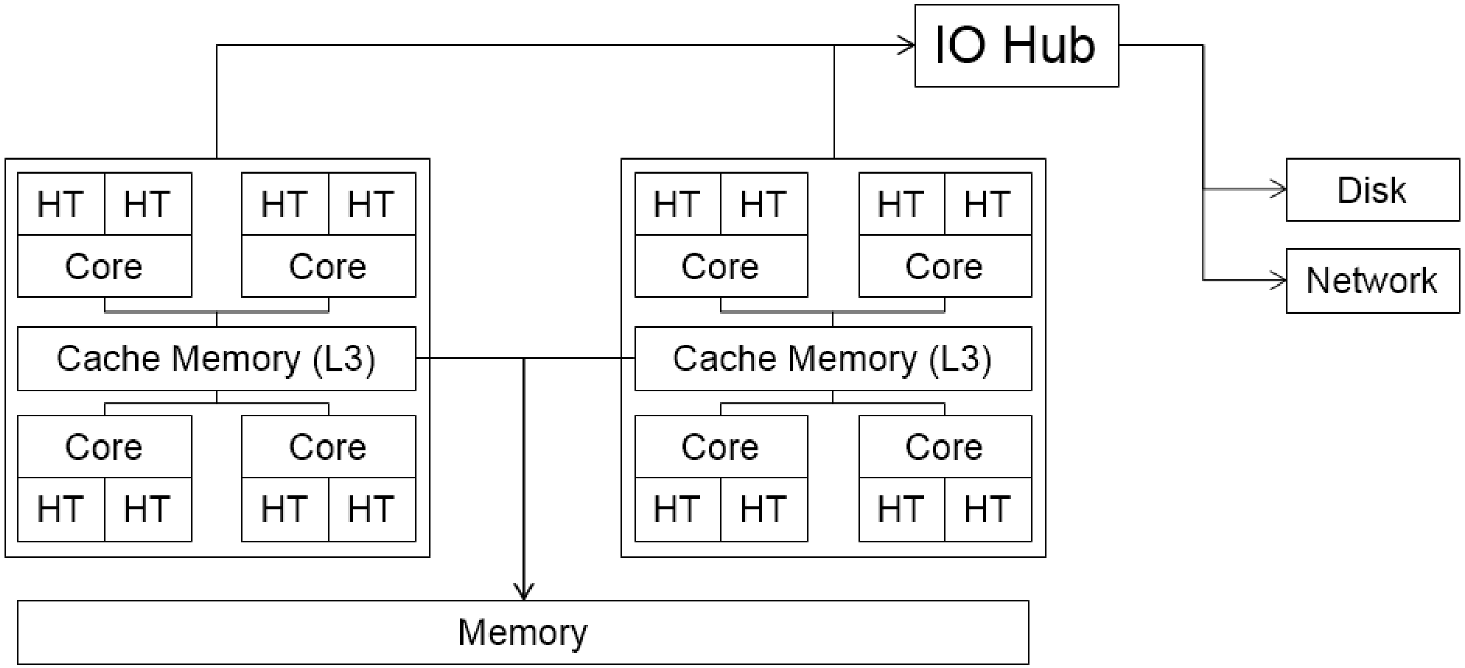
- Consider
  - Data transfer
  - Resource contention
  - Other overheads

Data Transfer

- `parfor` (Variable classification)
  - Broadcast goes once to each worker (what is actually accessed?)
  - Sliced sends just the slice (is all of the slice accessed?)
  - Reduction is sent back once per worker (usually efficient)

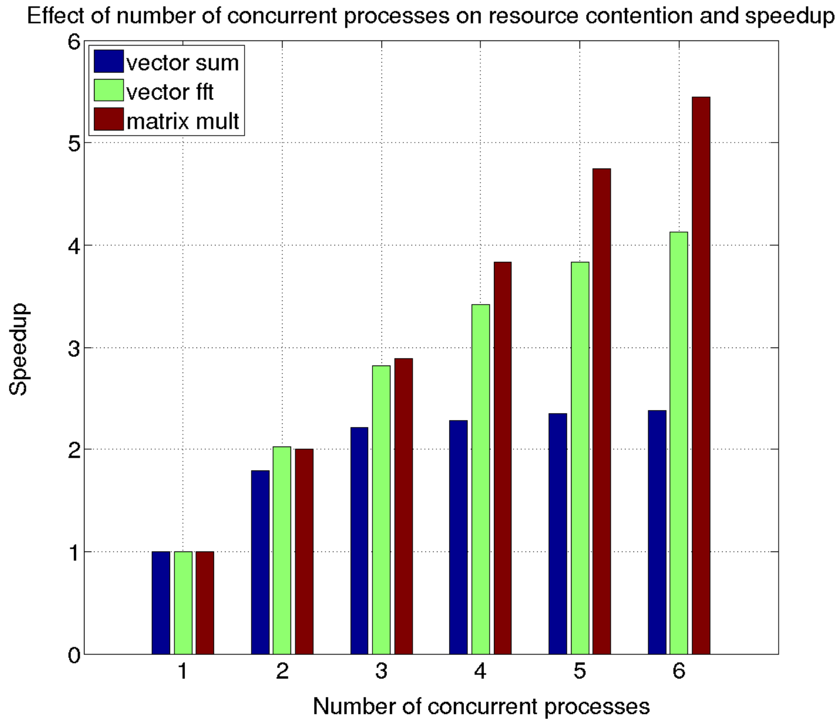
- `parfeval`
  - All inputs for a given call are passed to that worker

Resource Contention



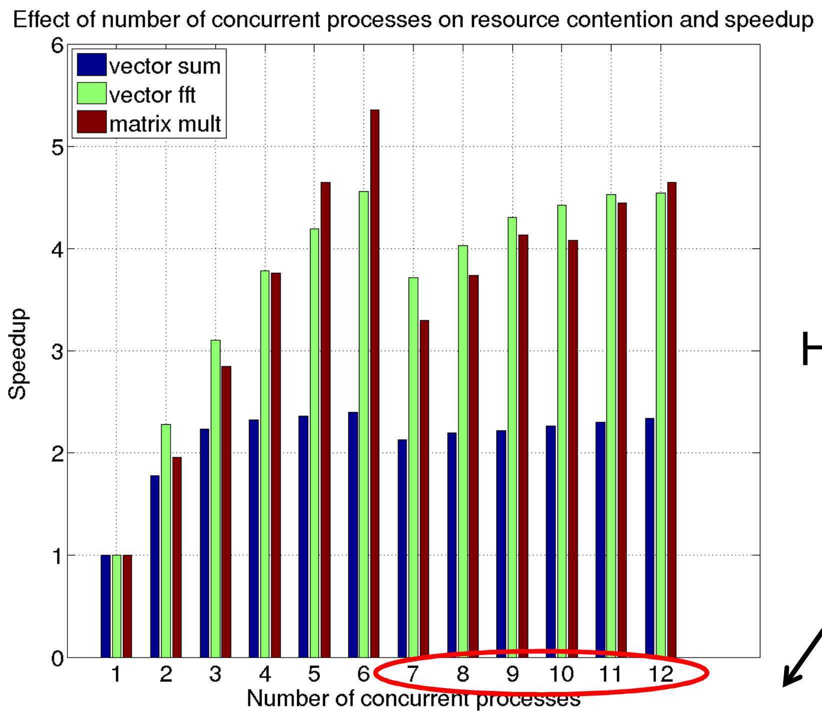
Speedup vs. num. Concurrent Processes

```
a = bigMatrix
    a*a
    fft(a)
    sum(a)
```



Speedup vs. num. Concurrent Processes

```
a = bigMatrix
    a*a
    fft(a)
    sum(a)
```



Hyperthreaded Cores

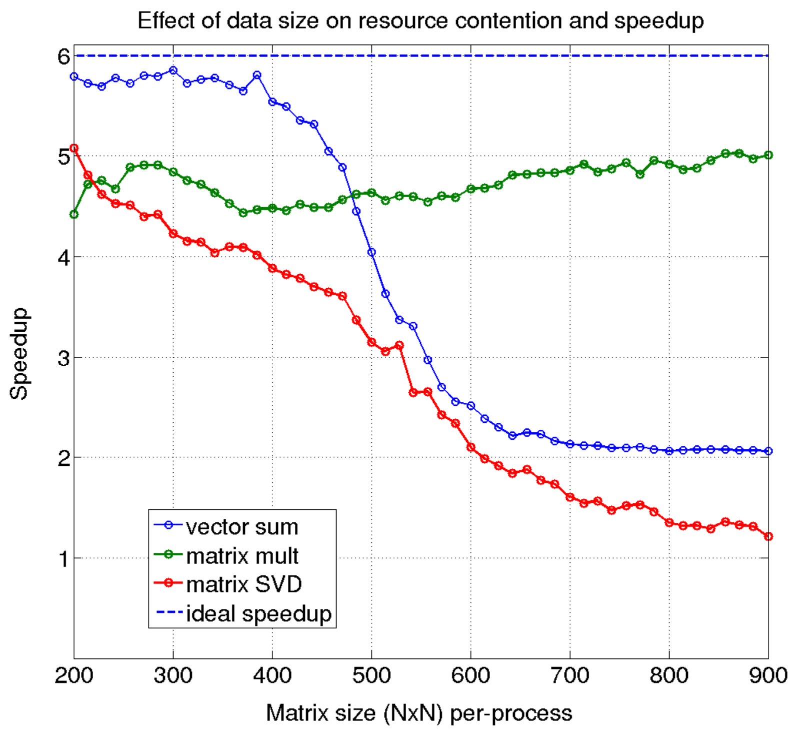
Speedup vs. Size of Data (6 procs.)

```
a = matrix(N)

    a*a

    sum(a)

    svd(a)
```



Summary (par*)

- Find enough parallelism
  - Go parallel as soon as possible
  - But not too small with **parfeval**

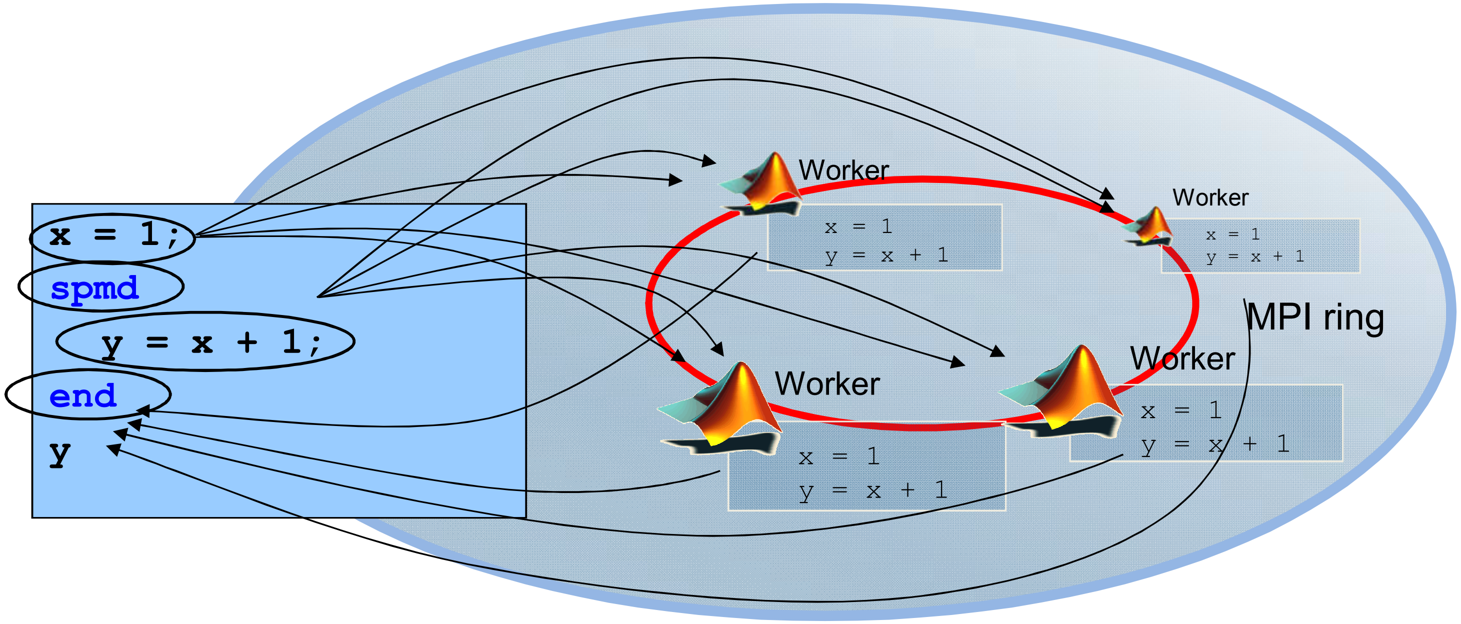
- Know how much data is being sent
  - Try to send as little as possible
- Understand how multiple algorithms might interact
- Keep workers busy if possible

Single Program, Multiple Data (spmd)

- Everyone executes the same program
  - Just with different data
  - Inter-lab communication library enabled
  - **labindex** and **numlabs** available to distinguish labs
- Example

```
x = 1
spmd
   y = x + labindex;
end
```

A Mental Model for `spmd . . . end`



Pool of MATLAB Workers

Common Parallel Program

```
forever {
    results = independentStuff( params )
    if results are OK {
        break
    } else {
        params = chooseNewParams( results, params )
    }
}
```

Solve with parfor

```
forever {
    parfor ii = 1:N {
        results(ii) = independentStuff( params(ii) )
    }
    if results are OK {
        break
    } else {
        params = chooseNewParams( results, params )
    }
}
```

Solve with spmd

```
spmd { forever {
    // Each of the workers computes its results (mine)
    results = gcat(independentStuff( params(mine) ))
    if results are OK {
        break
    } else {
        params = chooseNewParams( results, params )
    }
}}
```

spmdDemo

Summary (`spmd`)

- Required if inter-worker communication is needed for the algorithm
- Can provide better performance for some algorithms

GPUs

- Highly threaded
  - 10^6 threads not uncommon
- Very fast memory access
  - 200GB/s (~8x best CPU)
- Peak performance (double)
  - 1TFlop (~3x best CPU)

Getting data to the GPU

- To make an array exist on the GPU

```
g = gpuArray( dataOnCpu );
g = zeros( argsToZeros, 'gpuArray' );
g = ones( argsToZeros, 'uint8', 'gpuArray' );
```

- Supported types
  - All built-in numeric types

    `[complex|][[uint|int][8|16|32|64]|double|single]`

Using `gpuArray`

- Honestly – it's just like an ordinary MATLAB array
- Except that the methods that are implemented for it will run on the GPU (over 200 currently and growing)
  - Maybe some of these will be faster on your GPU

- Want to get the data back to the CPU

```
c = gather(g);
```

GPUness spreads

```
function [a, b, c] = example(d, e, f)

a = sin(d) + e;
b = cos(d) + f;
c = a + b + e + f;
```

GPUness spreads

```
function [a, b, c] = example(d, e, f)
% Imagine if the input d were on the GPU
a = sin(d) + e;
b = cos(d) + f;
c = a + b + e + f;
```

Getting data in the right place (new in 13b)

```
sIn = size(in);
out = in * eye(sIn) + ones(sIn);
```

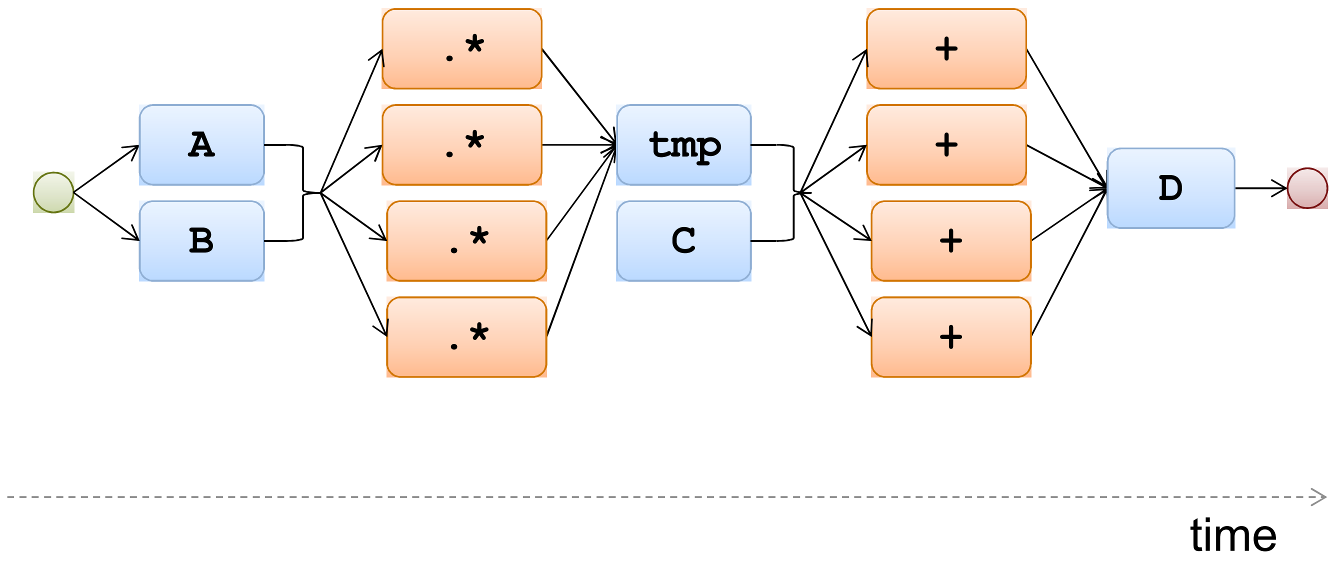
- The problem is that **eye** and **ones** make data in CPU memory
  - And so we need to transfer data to the GPU (which is *relatively slow*)

```
out = in * eye(sIn,'like',in) + ones(sIn,'like',in);
```

- **'like'** says make the data in the same place and as the same type as the prototype provided

Semantic work pattern: `gpuArray`

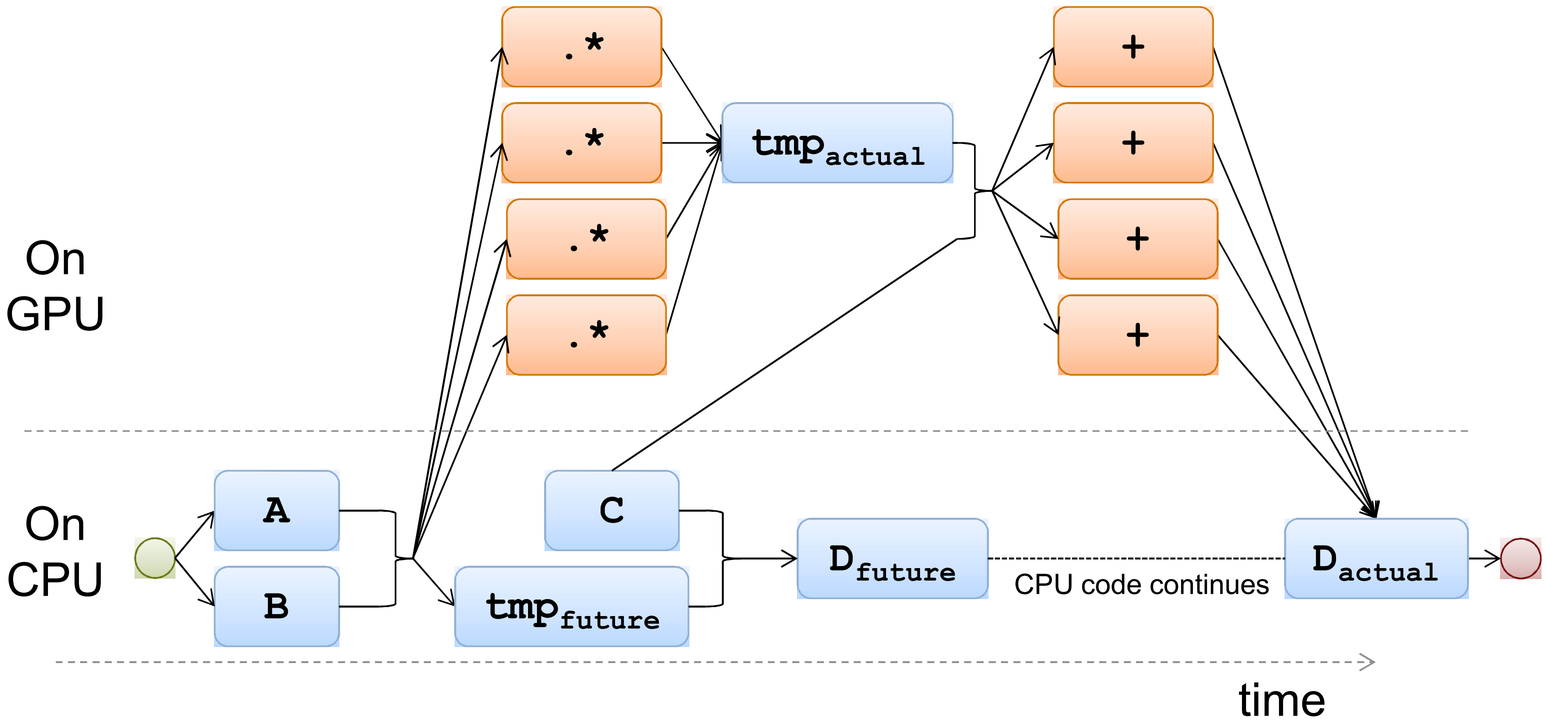
`D = A.*B + C`



Lazy Evaluation

- Where possible we queue things up on the GPU and return back to the program immediately
  - We also try to amalgamate sets of operations together

Actual work pattern: `gpuArray`



Lazy Evaluation

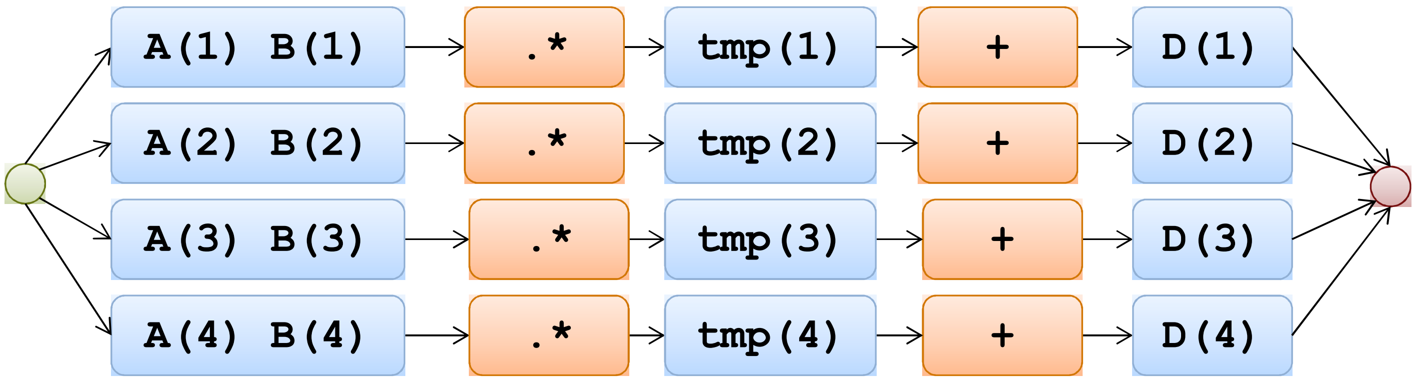
- Why do you care?
  - Improves performance a lot
  - CPU & GPU work at the same time.
- But be careful because **`tic;toc;`** can easily give you the wrong time, since the computation hasn't finished

```
d = gpuDevice; % Get the current GPU device
tic
    gpuStuffToTime;
    wait(d); % wait for computation on the GPU d to finished
toc
```

Can we do better?

GPU

```
D = A.*B + C
```



arrayfun

- Apply a function to each element of a set of gpuArrays

```
[o1, o2] = arrayfun(@aFunction, s1, s2, s3)
```

- Some limitations apply
  - All code uses scalar variables
  - Only a subset of the MATLAB language is supported

Why is this a good idea?

- We know what inputs are being passed to your function
- We know what code is in your function

- *with that* we can infer the type of all variables in your code

- *and then* we can generate code for your GPU

- for each element of your input arrays we can execute your function on a single CUDA thread
  - remember a GPU can execute thousands of threads at once, and schedule even more

```
gpuMandelbrotDemo
```

Singleton Expansion

Whenever a dimension of an input array is singleton (equal to one), we virtually replicates that array along that dimension to match the other arrays.

– *scalar expansion* is a specific instance of **singleton expansion**

Look for functions that support singleton expansion (**`arrayfun`**, etc.)

```
singletonExpansionDemo
```

Batching many small operations (`pagefun`)

- You have many matrices held in the pages of a multi-dimensional array
- You want to carry-out the same operation on each of the individual pages of the big array e.g.

```
for ii = 1:numPages
    C(:,:,ii) = A(:,:,ii) * B;
end
```

```
gpuPagefunDemo
```

Invoking CUDA Kernels

MATLAB

```
% Setup
kern = parallel.gpu.CUDAKernel('myKern.ptx', cFcnSig)

% Configure
kern.ThreadBlockSize=[512 1];
kern.GridSize=[1024 1024];

% Run
[c, d] = feval(kern, a, b);
```

C & mex

```
// Setup
mxGPUArray const * A = mxGPUCreateFromMxArray(prhs[0]);
// Create a GPUArray to hold the result and get its underlying
// pointer.
mxGPUArray * B = mxGPUCreateGPUArray(mxGPUGetNumberOfDimensions(A),
                        mxGPUGetDimensions(A),
                        mxGPUGetClassID(A),
                        mxGPUGetComplexity(A),
                        MX_GPU_DO_NOT_INITIALIZE);
double * d_B = (double *)(mxGPUGetData(B));
// Standard CUDA kernel call using the CUDA runtime.
TimesTwo<<<blocksPerGrid, threadsPerBlock>>>(d_B, N);

}
// Device code prototype ...
void __global__ TimesTwo(double * const B, int const N) { ... };
```

Summary (GPU)

- Vectorize as much as possible
- Performance better for larger arrays (overhead smaller)
- Keep data on the GPU as long as possible
- Look for opportunities to use **`arrayfun`** and **`pagefun`**
  - Particularly some loops can become serial calls to these functions
  - Use less memory with singleton expansion