Charon: linear algebra made easy

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My story

1. Quantum computing!
2. Can we build a reliable memory for quantum bits?
3. Numerical simulation of quantum systems
4. New algorithms for quantum simulations
5. Can they be made to scale?

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Let's do it!

- Tools we need:
  - Tensor I/O
  - Tensor contractions
  - Singular Value Decompositions (SVDs)
  - Minimum eigenvalue solving
- Tools we have:
  - MPI Parallel I/O
  - Global Arrays
  - SciLAPACK
  - ARPACK
- Problems:
  - Incomplete!
  - Cumbersome to use!
    - Lots of boilerplate and plumbing code needed
    - Synchronous communication model

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The Vision

A parallel linear-algebra intensive code should not be more complicated than the algorithm being implemented.

A Simple Example

1. Read in an array
2. Increment all entries in the array by 1
3. Sum all of the entries in the array
4. Divide all entries in the array by the sum
5. Write out the array

A Simple Example

```
DistributedArray<float,1> A(16,1<<20);
A.loadFrom("infile");
A += 1;
float s = A.sum();
A /= s;
A.writeTo("outfile");
```

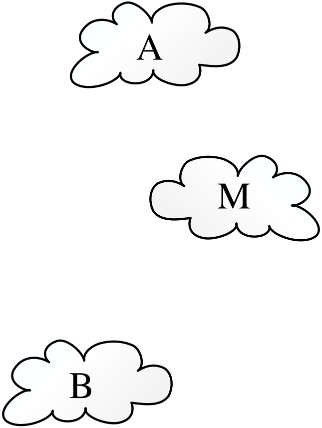
A More Complicated Example

1. Read in matrices A and B
2. Invert A and B
3. Multiply them together to form M
4. Break M apart back into A and B using a SVD
5. Invert A and B again
6. Save A and B

A More Complicated Example

```
DistributedArray<float,2> A(8,1024,1024),
    B(8,1024,1024), M(16,1024,1024);
DistributedArray<float,1> Sigma(16,1024);
A.loadFrom("A.in"); B.loadFrom("B.in");
inv(A); inv(B);
matmul(A,B,M);
svd(S,A,Sigma,B);
inv(A); inv(B);
A.writeTo("A.out"); B.writeTo("B.out");
```

Maestro, please!



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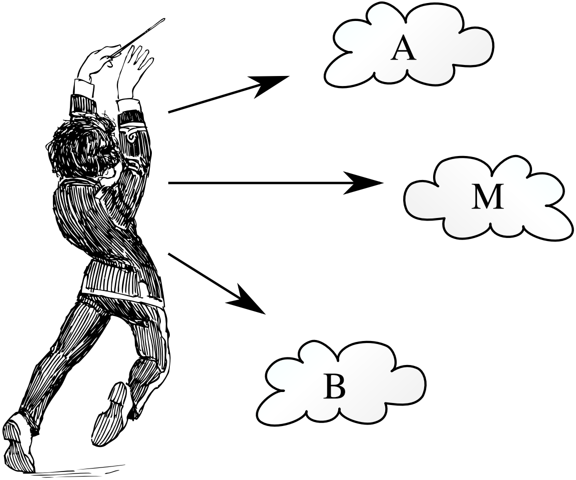

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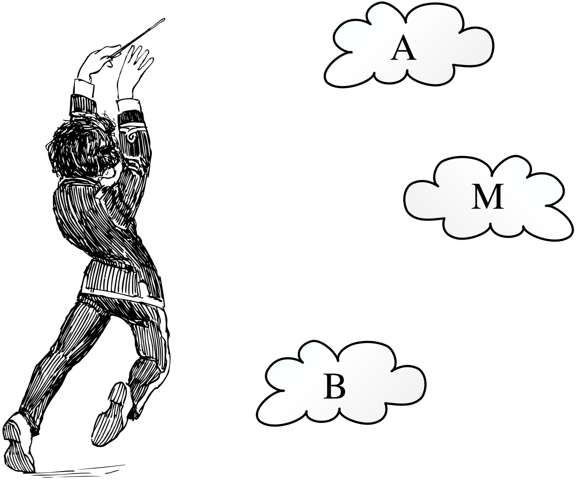

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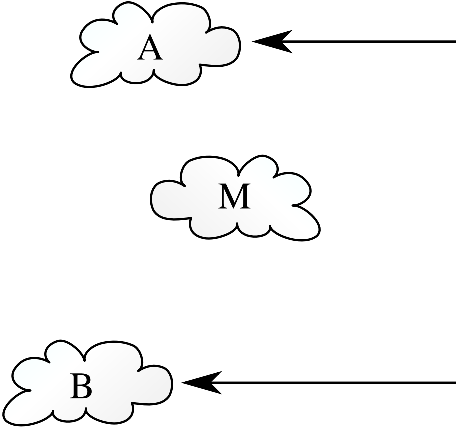

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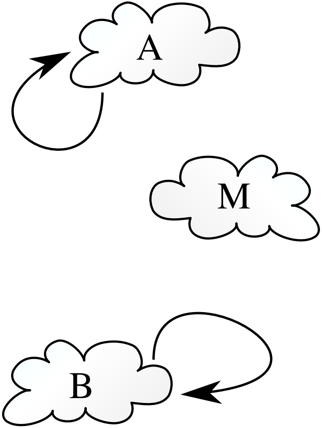

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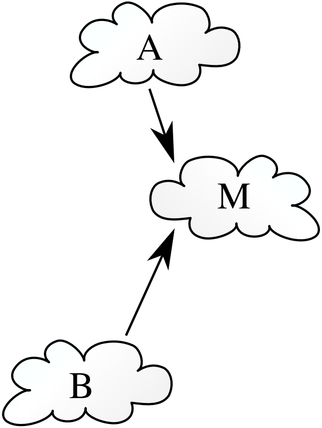

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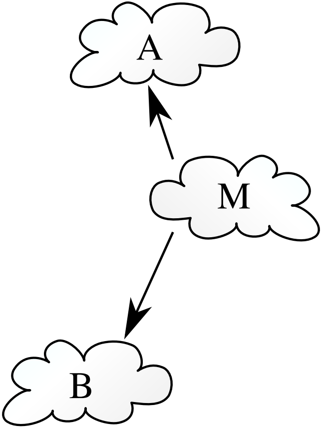

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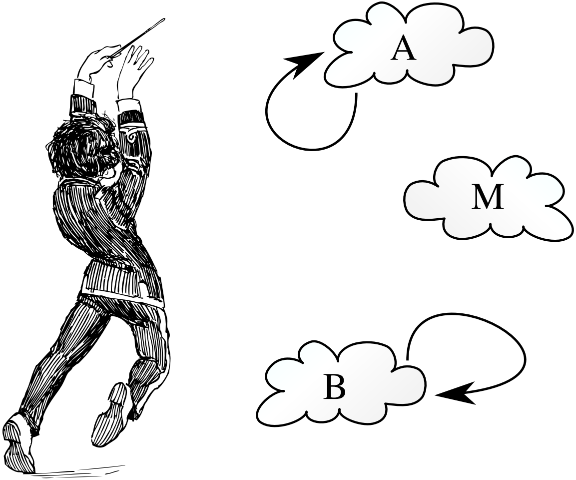

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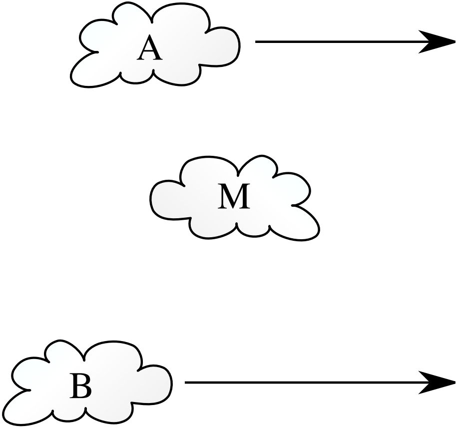

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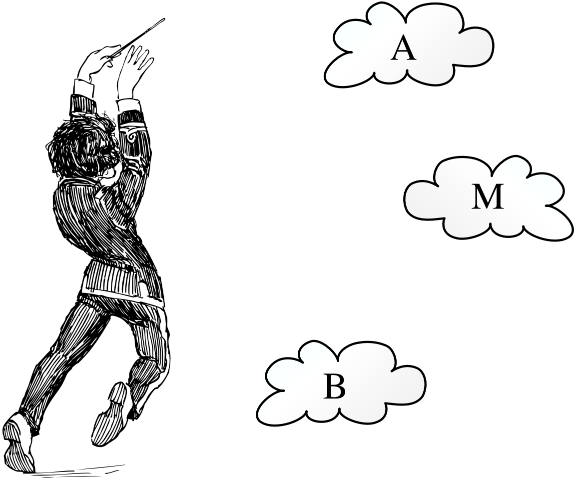

The Recipe

Ingrediants:

- Asynchronous communication
- Master/Slave architecture
- Explicit ordering and data dependencies

The result:

- Local coordination of task scheduling
    - (Caveat: Central decisions)
- Automatic parallelization of parallel tasks

(Effectively building and walking a DAG.)

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The Components

- Array Master/Slave Controller
  - Distributed Array
  - Block-cyclic Array
- Operations
- AMPI Master/Slave Controller
  - BLACS Grid Master/Slave (interface to BLACS)
  - Block IO Master/Slave (interface to ROMIO)
- Matrix multiplier

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Array Master/Slave Architecture

Question: How do we enforce ordering of operations?

Answer: Operation counters + slave priority queues

Question: How do we implement the counter?

- Global counter for all slaves
  - Commands sent to single slaves waste bandwidth!
- Separate counter for each slave
  - Huge table needed to track counters!
  - Global operations can no longer be broadcasted!

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My solution: Global counter with “stealing”

- Every operation increments the global counter
- Single slaves may “steal” a value of the counter
- Broadcasts to all slaves contain a list of who stole the counter since the last broadcast. This way every slave knows which values they should skip and which they need to wait for.

Example:

1. Broadcast 1 $\rightarrow$ 1, []
2. Pointcast 2 to A
3. Pointcast 3 to B
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- Templated on *type* and *dimension*
- Master:
  - Operation ordering
  - Addressing – map from coordinates to slave number
- Slaves: (1D array)
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  - Local data stored using Blitz++, a high level array class templated on *type* and *dimension*

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Operations

- Whole-array transformations
  - add/subtract/divide/multiply by a constant
  - sine, cosine, absolute value
  - randomization
  - etc.
- Single-element transformations
- Array reductions (sum, product, etc.)

Stupidly easy to implement more:

- Add to one of my switch statements
- Subclass `Operation`

Templates are your friend!

- Don't need to case over the type of the array.
- Not limited to numeric types / operations!

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Example

```
DistributedArray<int,3> vec(6,2,3,4);
Array<int,3> x(2,3,4);

x = 1, 2, 3, 4,
    5, 6, 7, 8,
    9,10,11,12,

    -1,-2,-3,-5,
    -7,-9,-11,-13,
    -17,-19,-23,-29,
    -31,-37,-41,-43;

vec = x;
```

Example

```
vec++;
vec *= -1;

cout << "0,0,0 = " << (int)vec(0,0,0) << endl;

for(int i = 0; i < 2; i++)
    for(int j = 0; j < 3; j++)
        for(int k = 0; k < 4; k += 2)
            vec(i,j,k) *= -1;

vec.abs();

vec.gatherInto(x);
```

AMPI Controller

- Purpose: To allow access to libraries written in MPI
  - BLACS – opens the door to parallel linear algebra libraries such as ScaLAPACK
  - ROMIO – parallel I/O
- Contains no data itself
- Requires coordination but not ordering
- Uses TCharm to provide the virtual MPI layer
  - Slaves inherit from TCharm
  - Constructor launches the TCharm thread
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Privateer

Problem: Most C libraries are not designed to be multi-threaded! They assume that they have exclusive access to their global/static variables.

Solution: Replace all references to global/static variables with pointers into a thread-local structure.

Privateer accomplishes this, and is designed to work on arbitrary C code; it uses a Converse thread-private variable to store a pointer to the global variable table for the thread.

`http://launchpad.net/privateer`

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Matrix Multiplication

$$\sum_j \mathbf{A}_{ij} \cdot \mathbf{B}_{jk} = \mathbf{C}_{ik}$$

Chare (i, j, k) computes $\mathbf{A}_{ij} \cdot \mathbf{B}_{jk}$, and then contributes to a sum reduction on the section $(i, :, k)$.

Chunks sent in an `ArrayMessage` to minimize copying.

Each chare *only* needs to know

- Reduction section
- Result callback

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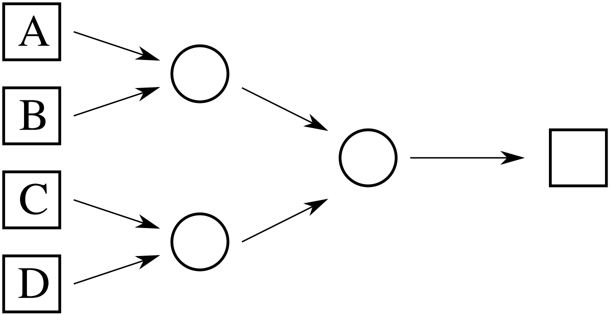
$$\mathbf{A} \cdot \mathbf{B} \cdot \mathbf{C} \cdot \mathbf{D} = (\mathbf{A} \cdot \mathbf{B}) \cdot (\mathbf{C} \cdot \mathbf{D})$$



Closing

Status:

- Basic infrastructure largely complete; lots of simple operations could easily be implemented
- Still wrestling with getting libraries to work under AMPI
  - (Global variable privatization problem has been solved by `Privateer`.)
- Need to profile matrix multiplication algorithm and extend to implement tensor contractions

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- `http://launchpad.net/charon`

Please let me know what you think and/or want!

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Repositories Online:

- `http://launchpad.net/privateer`
- `http://launchpad.net/charon`

Please let me know what you think and/or want!