Taming Complex Bioinformatics Workflows with Weaver, Makeflow, and Starch

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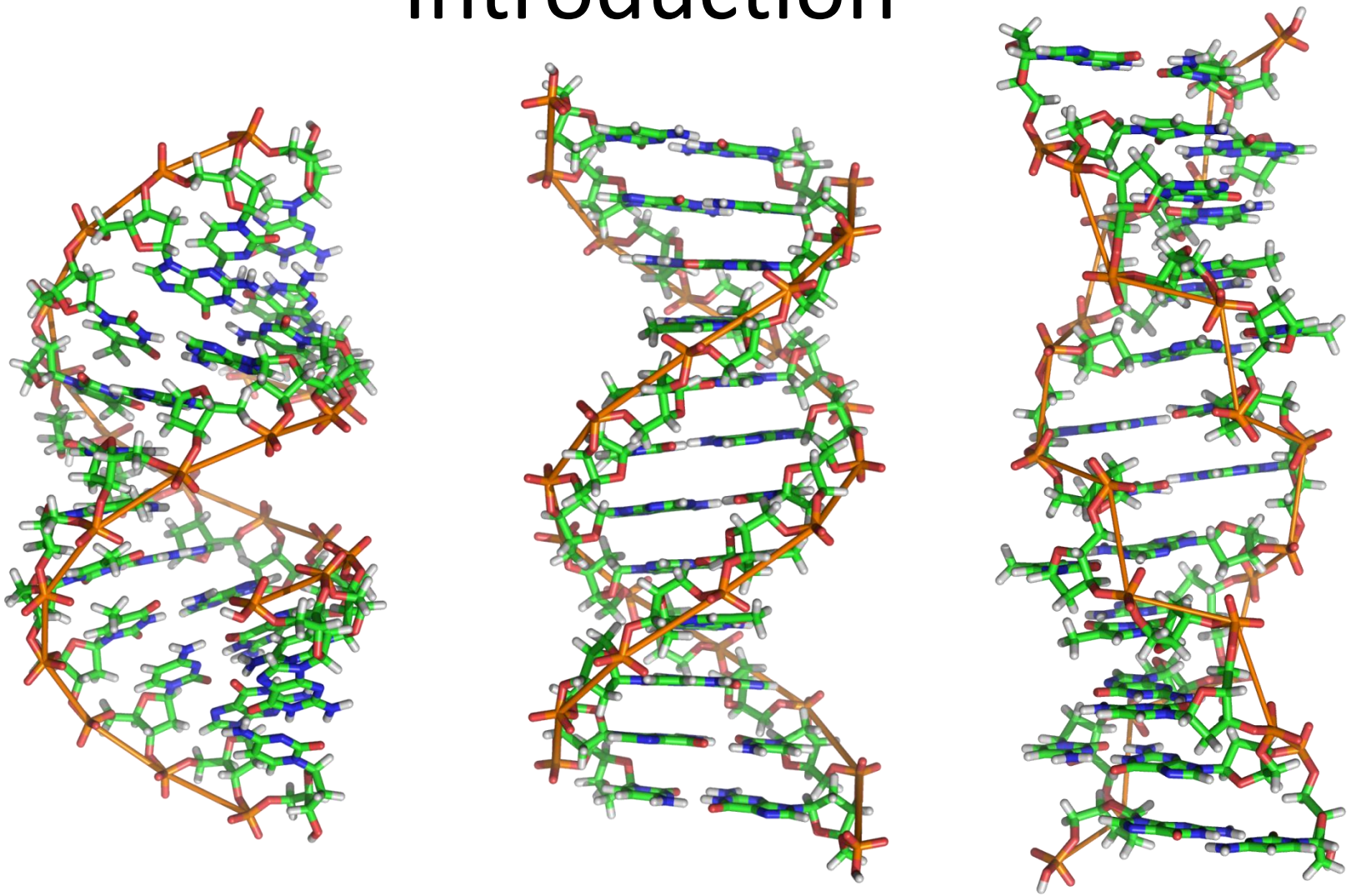
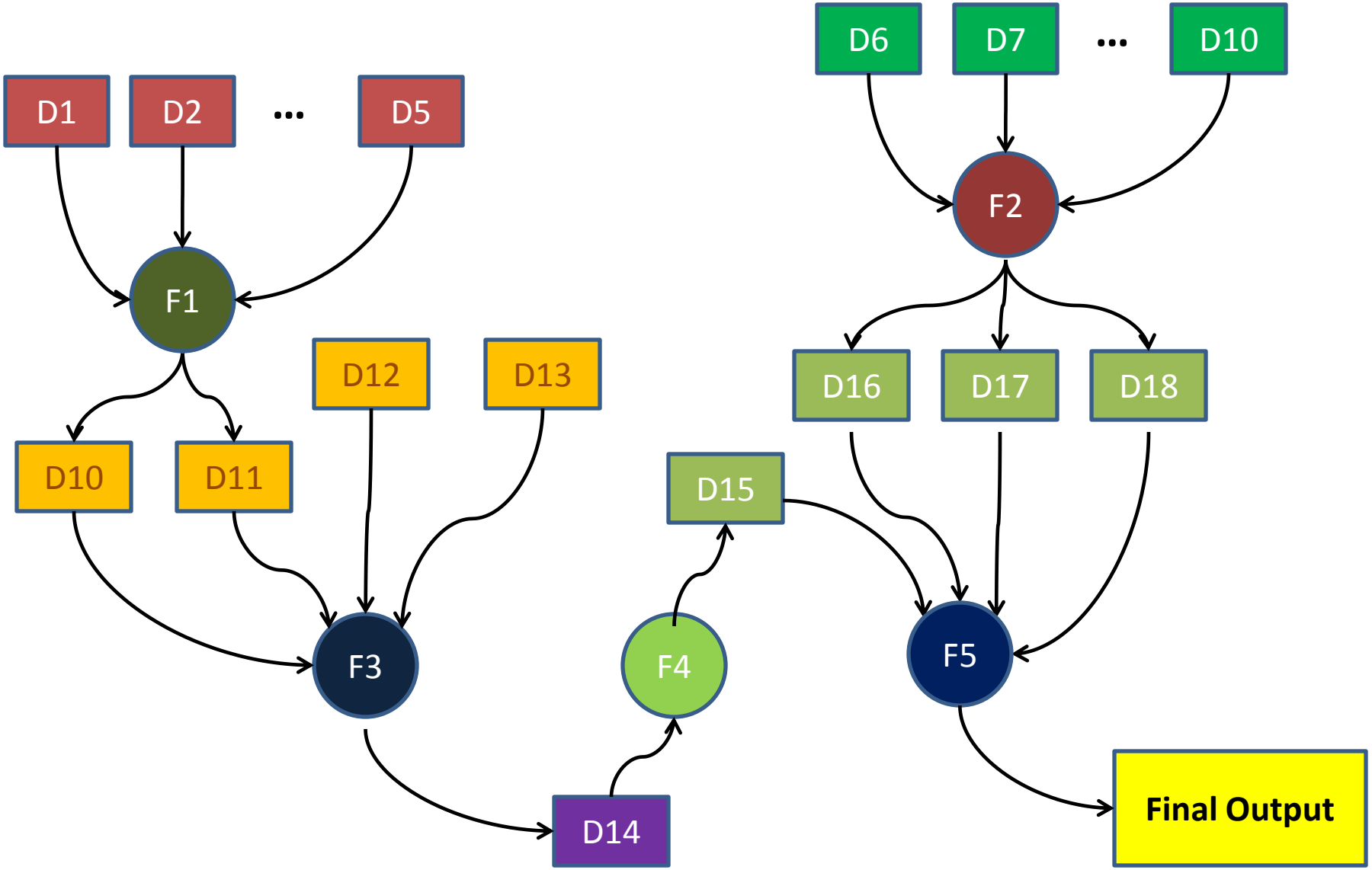
Introduction



Source: Wikimedia

Introduction

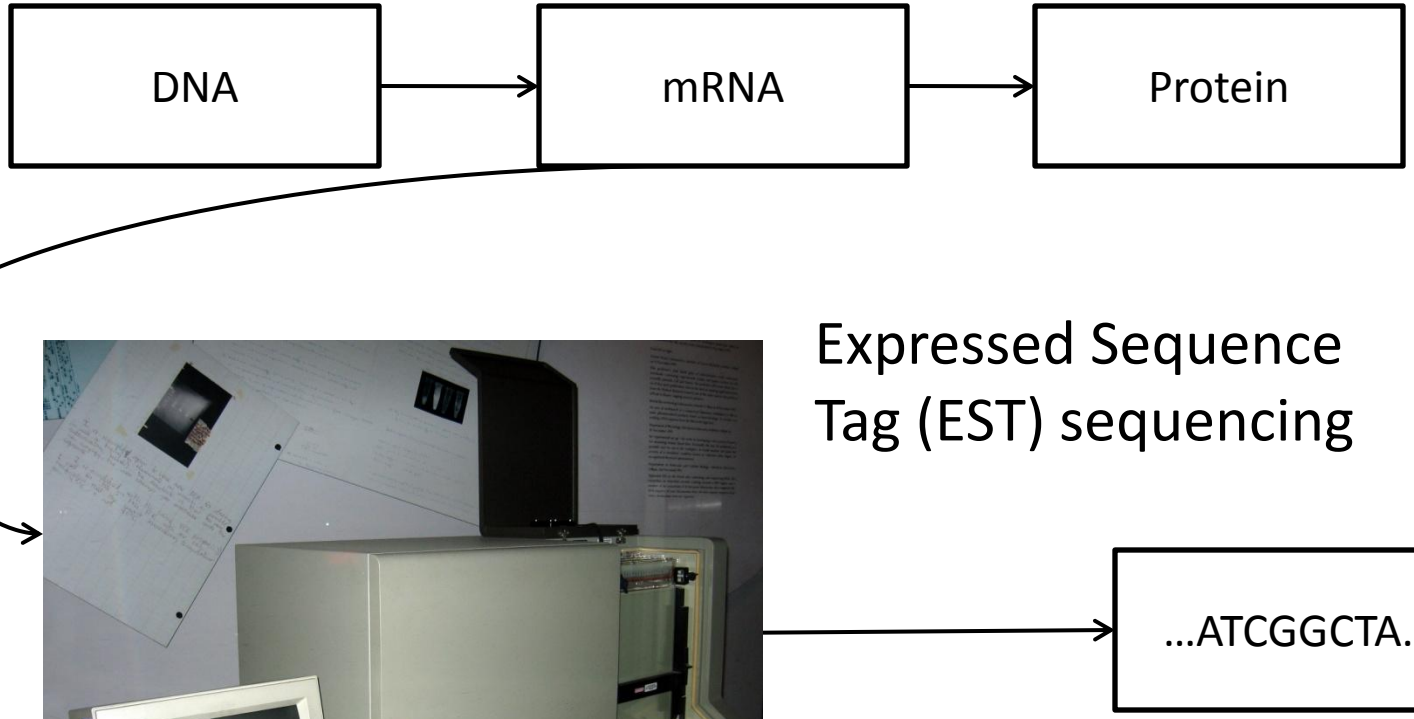


Challenges

- Portability
  - Designed for a particular system
- Software maintainability
  - Goals and hypotheses change over time
- Dependency management
  - Reliance on third party libraries and executables

EST pipeline

Protein Synthesis:



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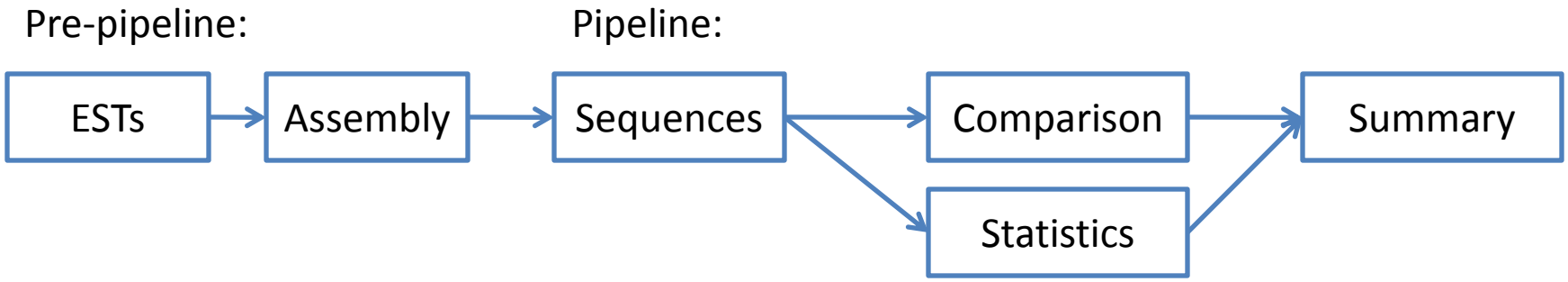
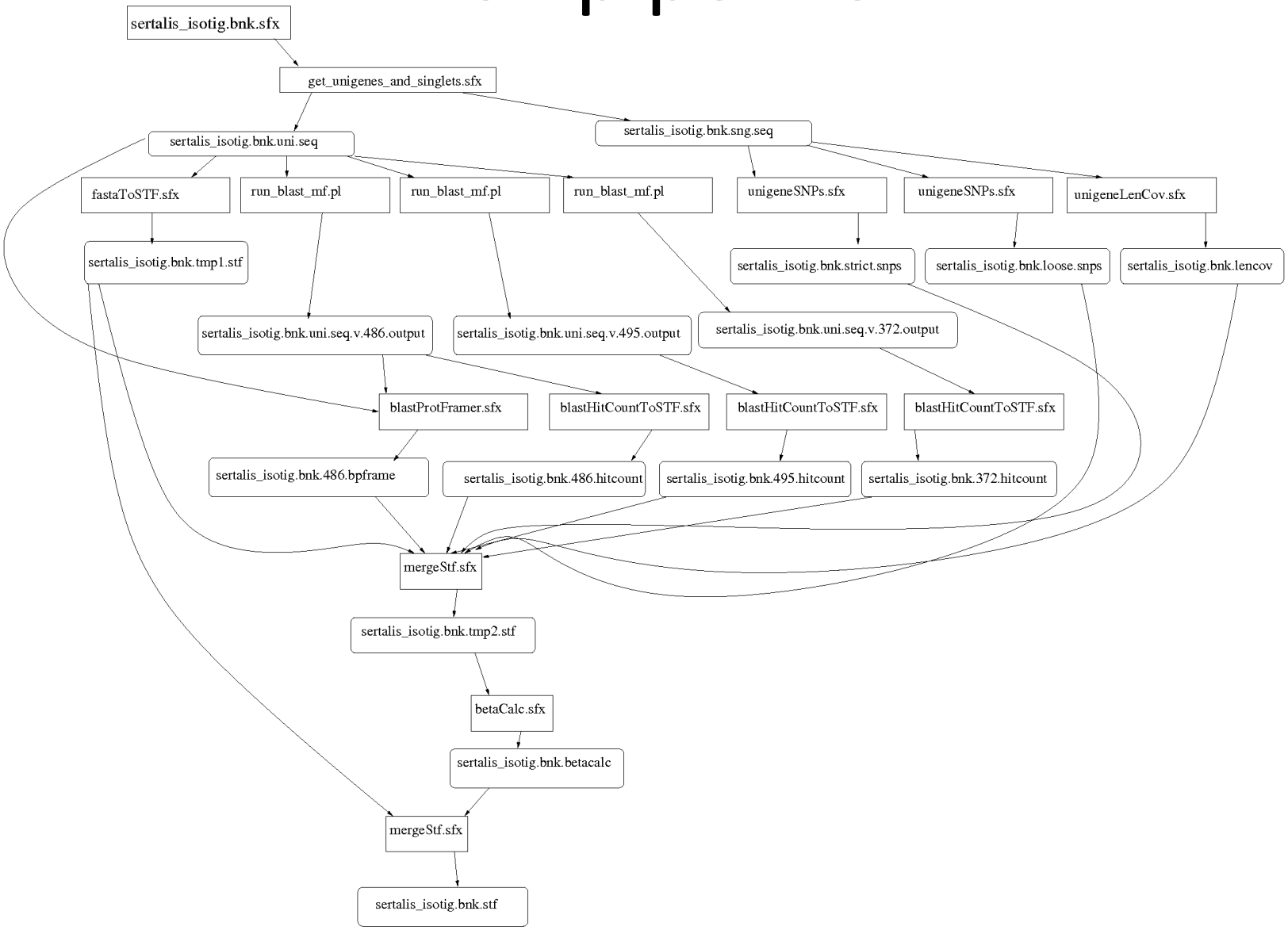
EST pipeline



EST pipeline

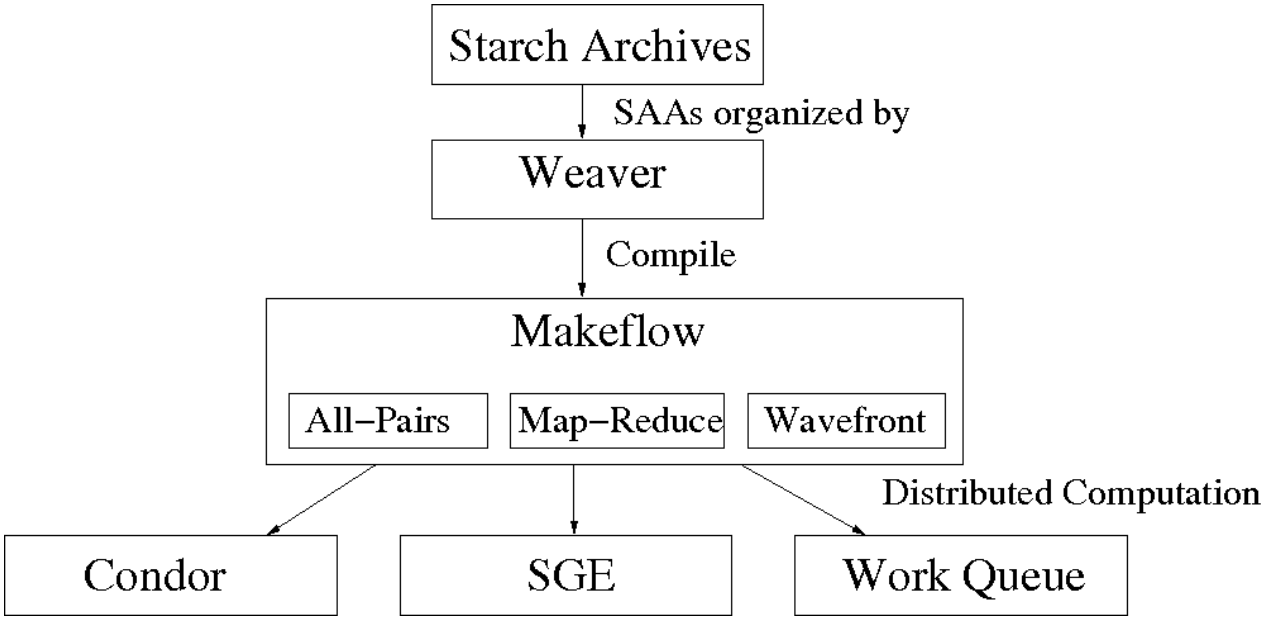


Solution Strategy

- Encapsulation of environment
- High level workflow specification language
- Portable low level workflow engine

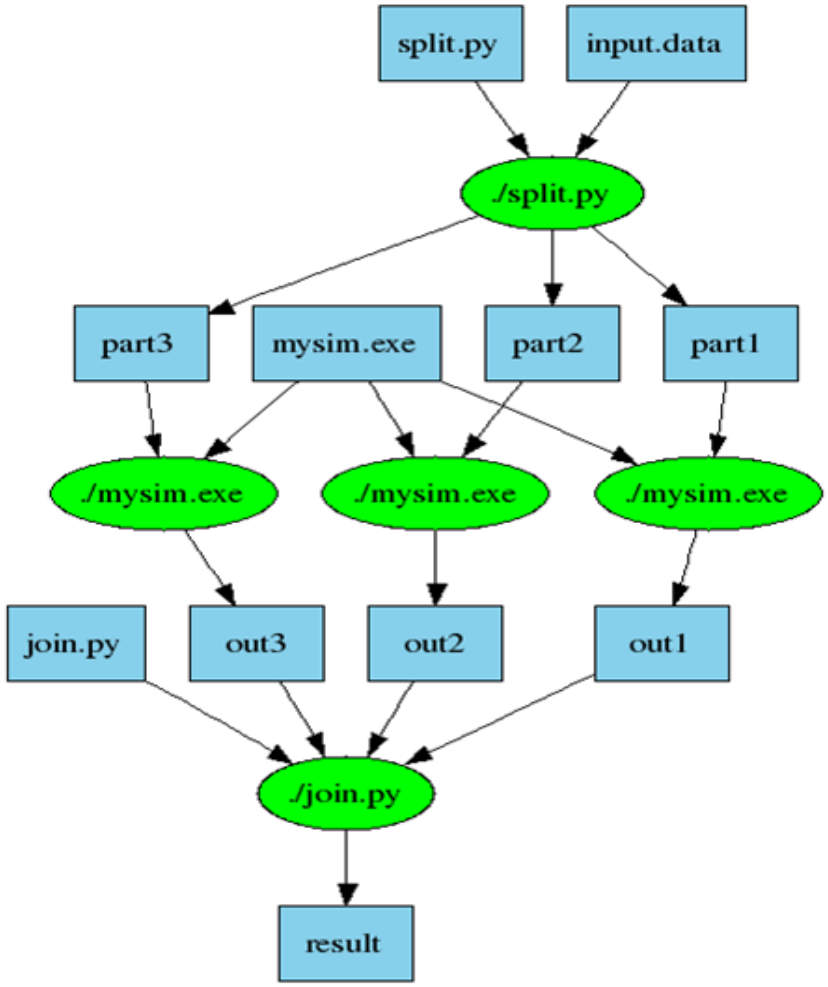
Solution Tools

- Starch
- Weaver
- Makeflow

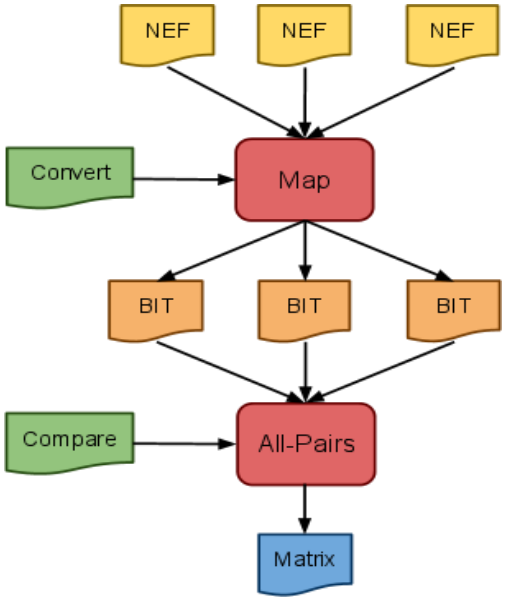


Solution Tools - Makeflow

```
part1 part2 part3: input.data split.py
        ./split.py input.data

out1: part1 mysim.exe
        ./mysim.exe part1 > out1

out2: part2 mysim.exe
        ./mysim.exe part2 > out2

out3: part3 mysim.exe
        ./mysim.exe part3 > out3

result: out1 out2 out3 join.py
        ./join.py out1 out2 out3 > result
```



Solution Tools - Weaver



General DAG

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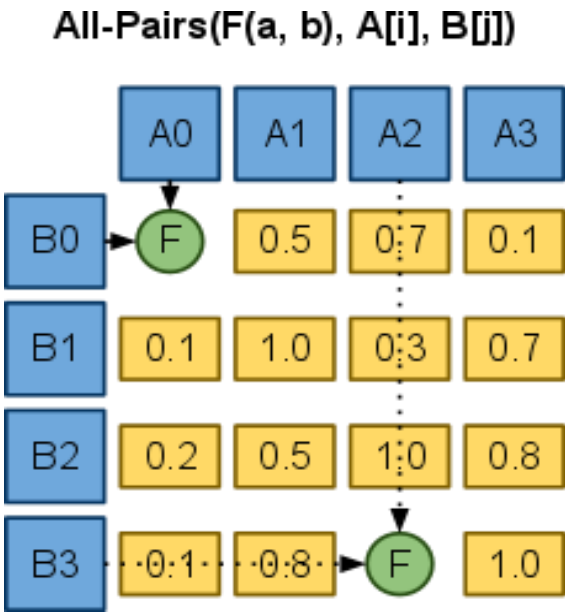

Specific Abstraction

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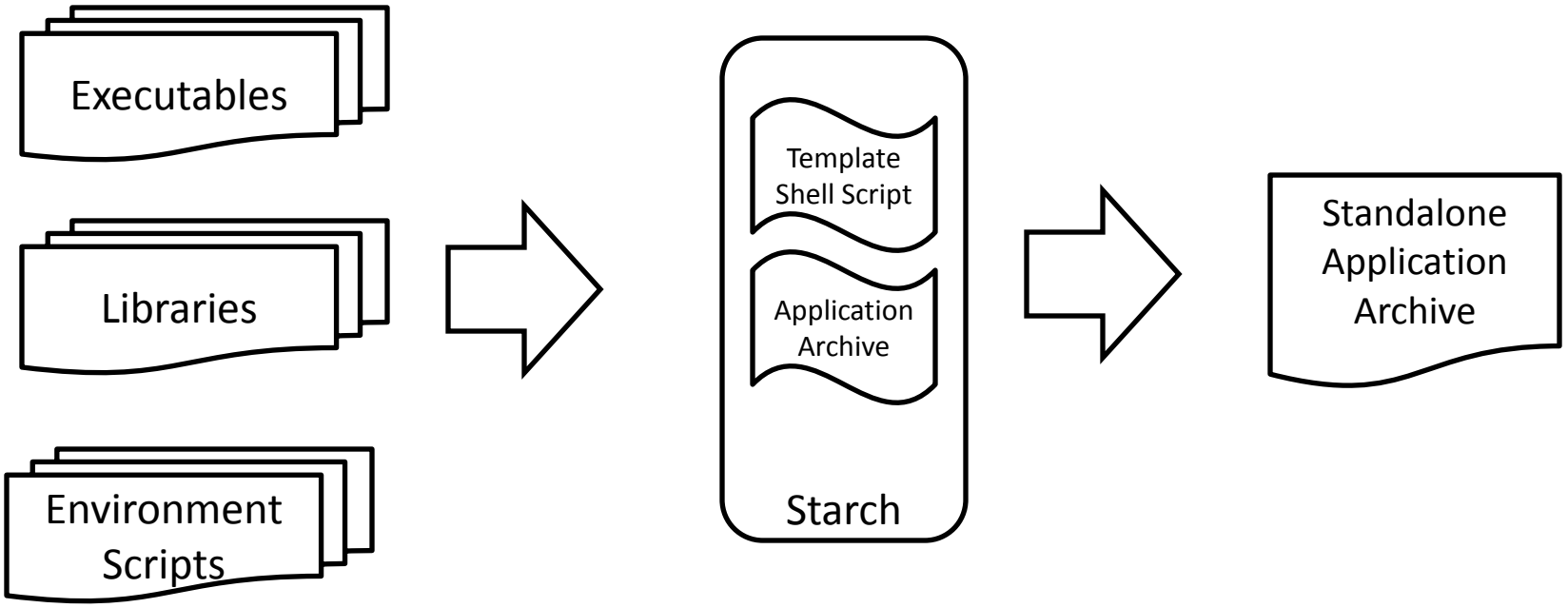
interface

=

Simplified Distributed Programming

Solution Tools - Starch



Final EST pipeline

Perl

```
print "$amosbnk.betacalc betacalc.err: betaCalc GeneticCode.rb $amosbnk.tmp2.stf ruby wrapper.pl
    $amosbnk.tgz bio.tgz bio-1.3.0.tgz ruby_gems-1.9.1.tgz bio.rb\n";
print "\t./wrapper.pl $amosbnk.tgz '(./ruby betaCalc $amosbnk.tmp2.stf ugAveCov seq maj_ugp_strict
    min_ugp_strict blastx_hsp MainStrict > $amosbnk.betacalc) >& betacalc.err'\n\n";
print "$amosbnk.stf stf.err: mergeStf $amosbnk.tmp1.stf $amosbnk.betacalc ruby wrapper.pl $amosbnk.tgz
    bio.tgz bio-1.3.0.tgz ruby_gems-1.9.1.tgz bio.rb\n";
print "\t./wrapper.pl $amosbnk.tgz '(./ruby mergeStf $amosbnk.tmp1.stf $amosbnk.betacalc > $amosbnk.stf) >&
    stf.err'\n";
```

Weaver

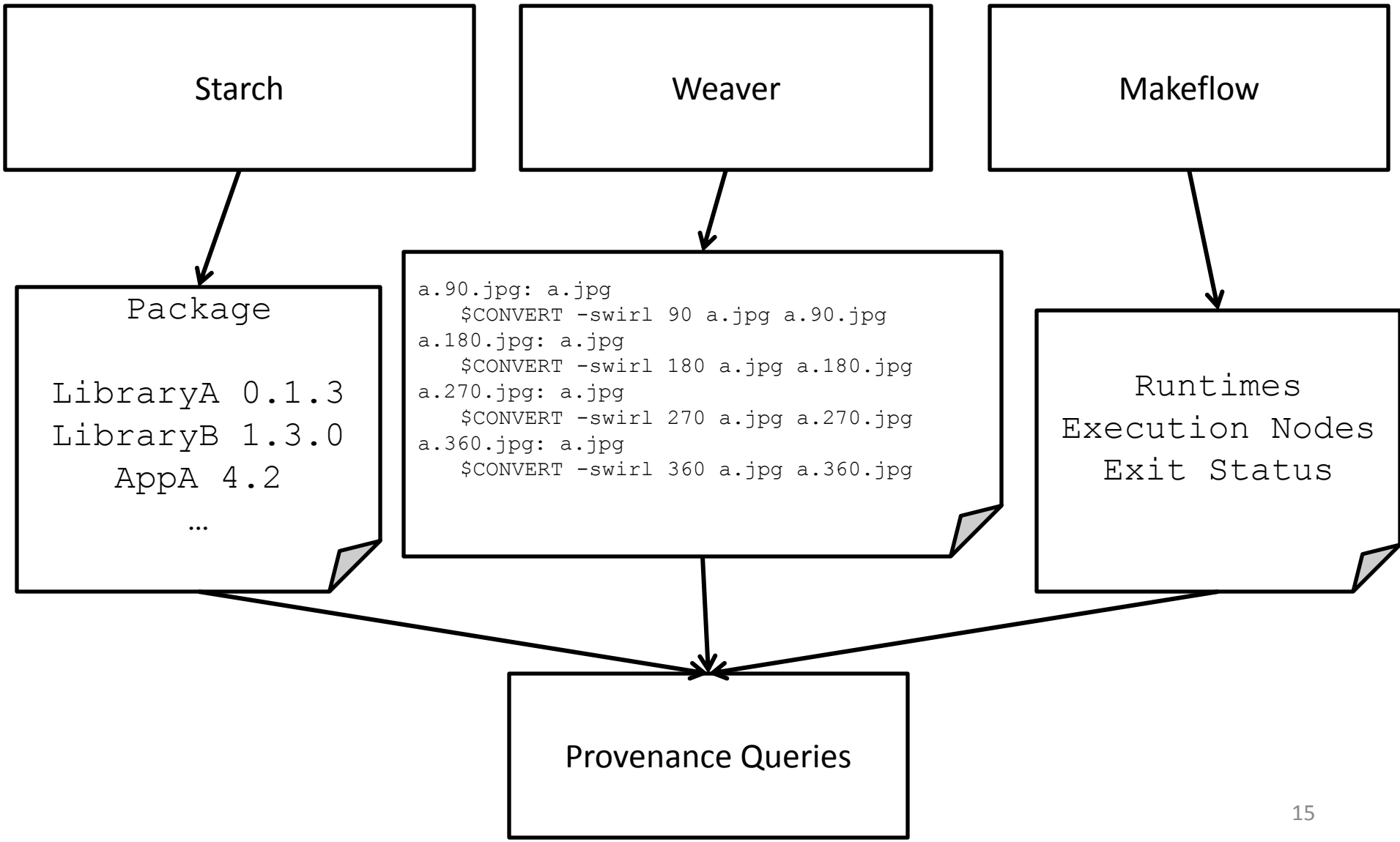
```
f = betaCalc(str(bank)+'.tmp2.stf ugAveCov seq maj_ugp_strict min_ugp_strict blastx_hsp MainStrict')
t = Run(f, '', output = f.output_string(str(bank)+'.betacalc'))

f = mergeStf(str(bank)+'.tmp1.stf '+str(bank)+'.betacalc')
t = Run(f, '', output = f.output_string(str(bank)+'.stf'))
```

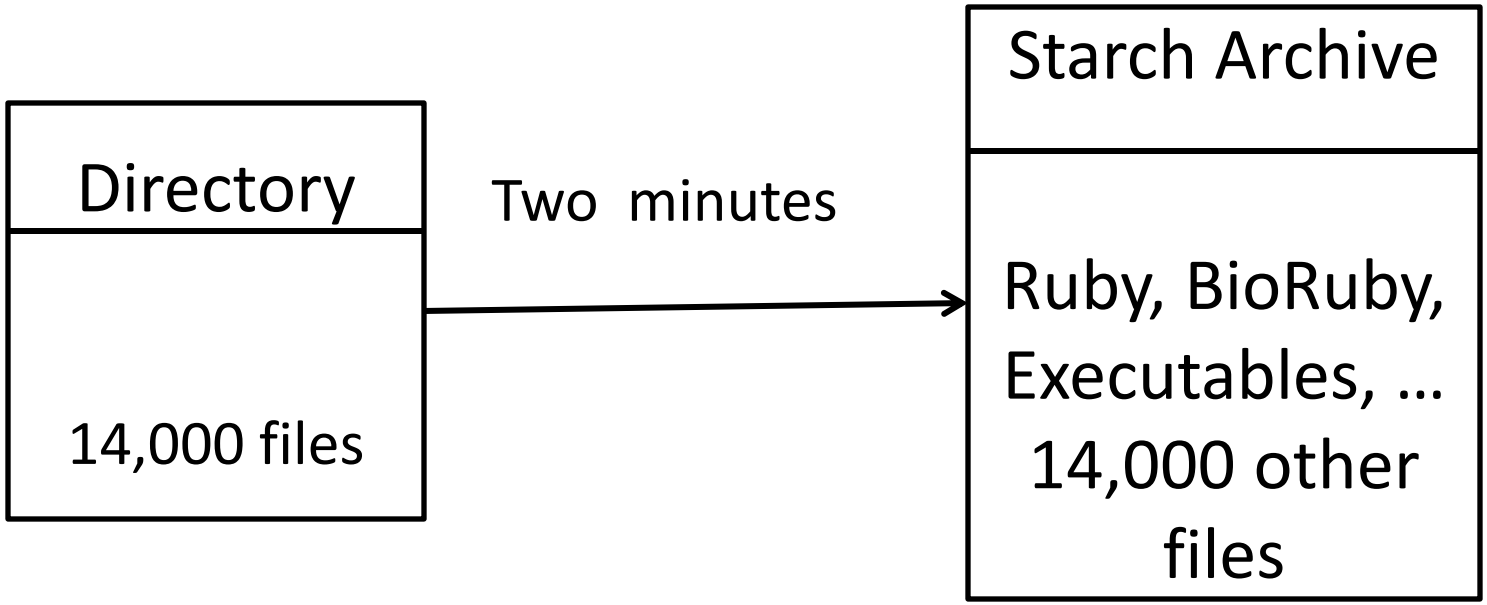
Pipeline Characteristics

- Provenance
- Encapsulation
- Performance
- Portability
- Fault Tolerance
- Code Clarity

Pipeline Characteristics - Provenance



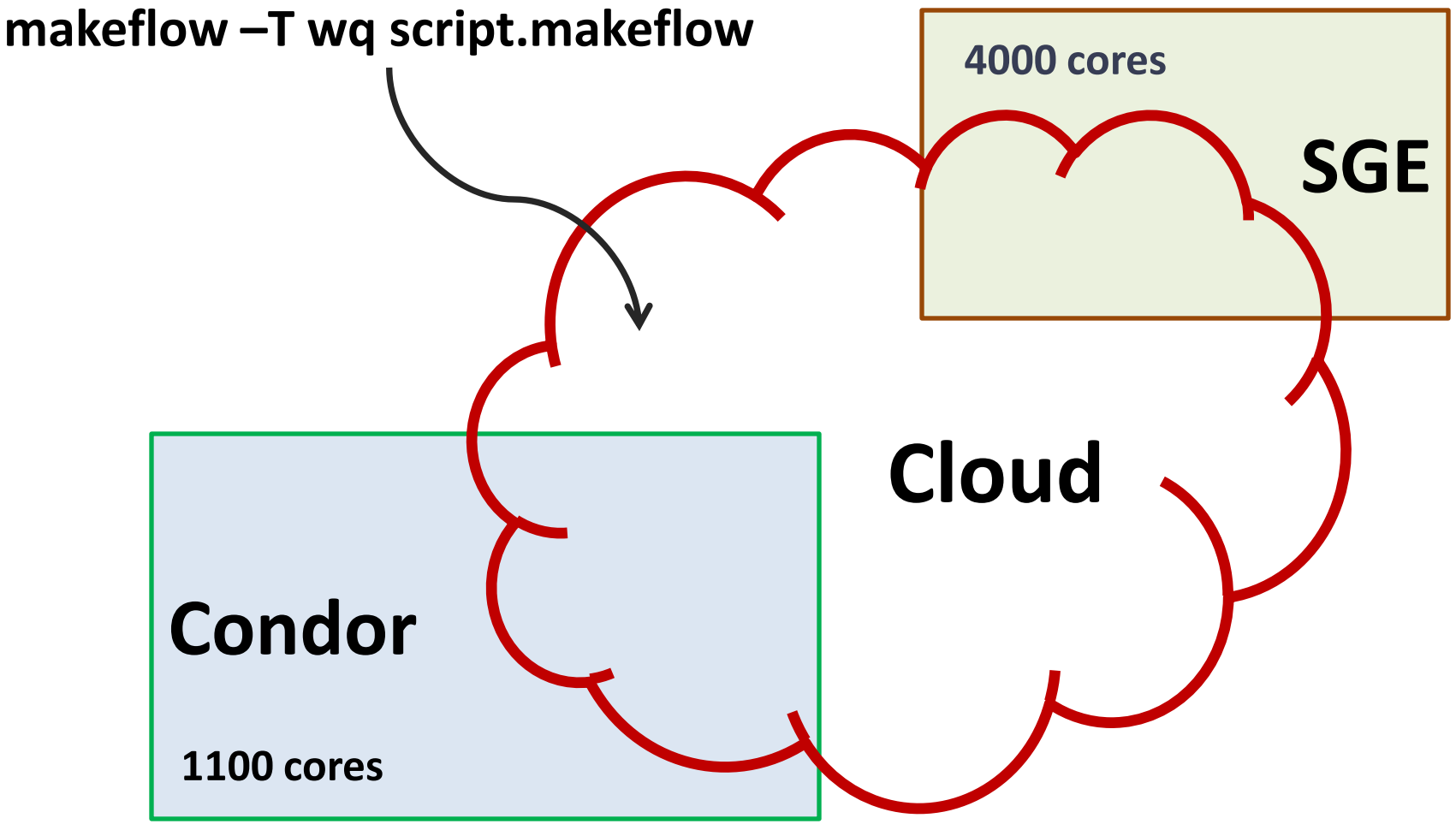
Pipeline Characteristics - Encapsulation



Pipeline Characteristics - Performance

- Manual (sequential execution) – 1 week
- Makeflow (automated execution) – 1 hour
- No difference in Perl and Weaver

Pipeline Characteristics - Portability



Pipeline Characteristics – Fault Tolerance

- Makeflow tracks job progress and supports automated rerunning failed tasks

- Makeflow can resume execution from stoppage

Pipeline Characteristics – Code Clarity

- Weaver generating a Makeflow

```
f = split(query, database)
t = Run(f, '', output = f.output_string(split_out), local = True)
Map(Blast, files, output = 'blast.output', merge_func = 'cat' )
```

- Perl generating a Makeflow

```
for (my $i = 0; $i < $num_splits; $i++) {
		$inputlist .= "$inputfile.v.$dbfile.input.$i ";
		$outputlist .= "$inputfile.v.$dbfile.output.$i ";
		$errorlist .= "$inputfile.v.$dbfile.error.$i ";}
print OUTFILE $inputlist . ": $inputfile split_inputs.pl\n";
print OUTFILE "\tLOCAL ./split_inputs.pl $qry_granularity $char_granularity $inputfile
$dbfile\n\n";

for (my $i=0; $i < $num_splits; $i++) {a
		print OUTFILE "$inputfile.v.$dbfile.output.$i $inputfile.v.$dbfile.error.$i:
$inputfile.v.$dbfile.input.$i $dbfile.tgz blastall tee blastwrapper.pl\n";
		print OUTFILE "\t./blastwrapper.pl $dbfile $inputfile $i\n\n";
```

Conclusion – Lessons Learned

- Code modularity
- Code clarity
- Abstractions
- Portability

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  - Shawn O'Neil
  - Rory Carmichael
  - Andrew Rider
  - Irena Lanc
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  - Peter Bui
  - Li Yu

Software

- Makeflow
  - http://www.nd.edu/~ccl/software/makeflow
  - or Google “Makeflow”
- Weaver and Starch
  - http://bitbucket.org/pbui/

Biocompute

http://biocompute.cse.nd.edu/