Declarative Infrastructure for Automated Scientific Computing

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Expertise

Domain knowledge is important for efficient computation

Expertise

Most scientific programmers aren't experts in all requisite domains

Expertise

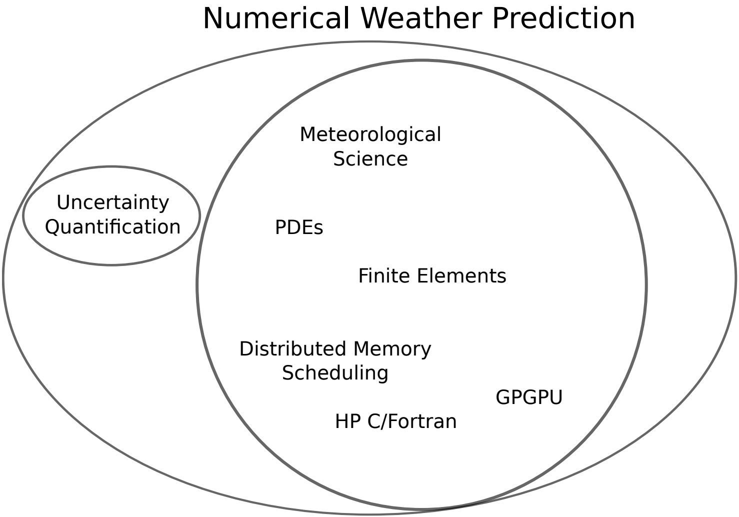
```c
// A: Naive
int fact(int n){
    if (n == 0)
        return 1;
    return n*fact(n-1);
}
```

```c
// B: Programmer
int fact(int n){
    int prod = n;
    while(n--)
        prod *= n;
    return prod;
}
```

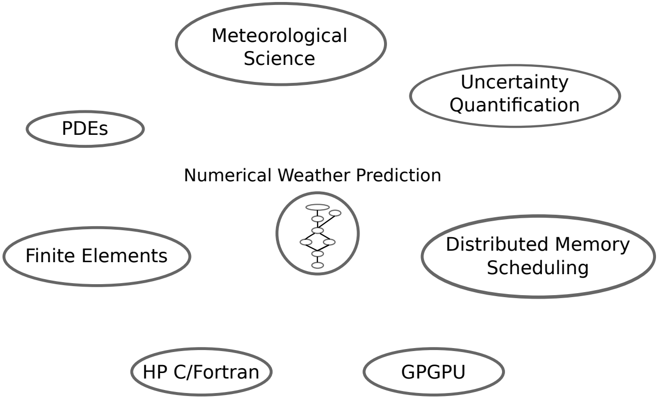
```c
// C: Mathematician
int fact(int n){
    // n! = Gamma(n+1)
    return lround(exp(lgamma(n+1)))
}
```

- Modern compilers automate B
- Humans do C by hand
- The people who know C are rarely trained to build compilers
- Both B and C are commonly necessary within one project

Composable Software - Monolithic



Composable Software - Composable



Outline

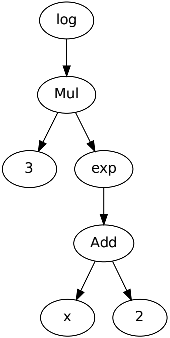
- Probability Modeling
  - Bayesian inference simulations (MCMC)
- Matrix algebra
  - BLAS/LAPACK computations
- Static Scheduling
  - Blocked Matrix Algorithms

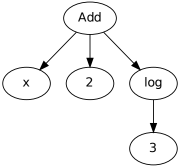
Section 1

Probability Modeling

Computer Algebra - SymPy

```
>>> expr = log(3*exp(x + 2))
>>> print simplify(expr)
x + 2 + log(3)
```

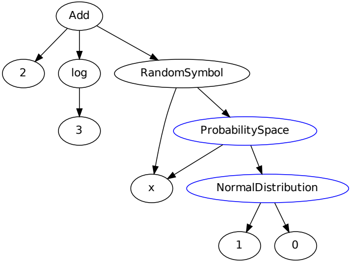




Random Variables

```
>>> x = Normal('x', 0, 1)

>>> expr = log(3*exp(x + 2))
>>> print simplify(expr)
x + log(3) + 2
```



Random Variables

```
>>> x = Normal('x', 0, 1)

>>> expr = log(3*exp(x + 2))
>>> print simplify(expr)
x + log(3) + 2

>>> P(expr > 4)
```

$$\int_0^{\infty} \frac{\sqrt{2} e^{-\frac{1}{2}(z - \log(3) + 2)^2}}{2\sqrt{\pi}}\, dz$$

1. Uncertainty doesn't interfere
2. Probability query $\rightarrow$ integral expression is a simple transformation
3. Integral problems have mature solutions

Random Variables

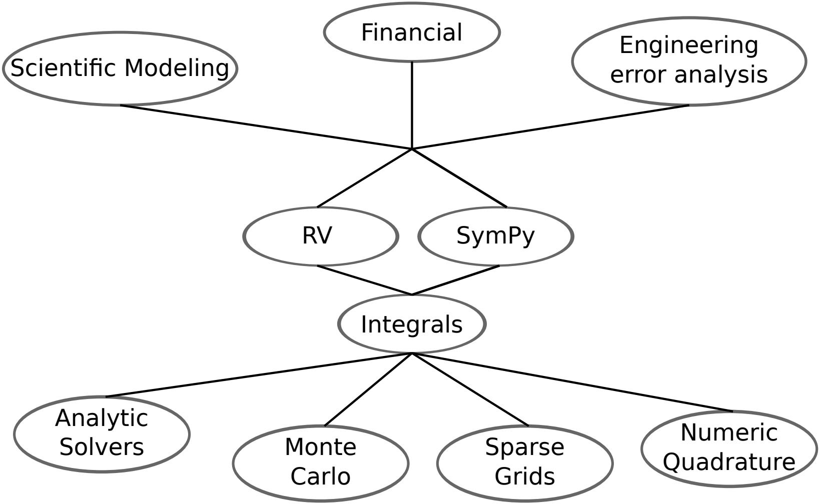


Figure:

Bayesian Inference

```
>>> rate = Beta('lambda', a, b)
>>> count = Poisson('count', rate)
```

$$p(x|\lambda) = \frac{\lambda^x}{e^\lambda x!} \qquad p(\lambda) = \frac{\lambda^{a-1} \left(-\lambda + 1\right)^{b-1} \Gamma\left(a + b\right)}{\Gamma\left(a\right) \Gamma\left(b\right)}$$

Infer `rate` given many observations for `count`

$$\text{Maximize} \quad p(\lambda|x_i) \propto \prod_i p(x_i|\lambda) \cdot p(\lambda)$$

$$0 = \frac{d}{d\lambda} \log \left(\prod_i p(x_i|\lambda) \cdot p(\lambda) \right) = \frac{d}{d\lambda} \sum_i \log(p(x_i|\lambda) \cdot p(\lambda))$$

Need to find the roots of

$$\sum_{i=1}^{n} \frac{a \left(\lambda - 1\right) + b\lambda - \lambda \left(\lambda - 1\right) - 2\lambda + \left(\lambda - 1\right) \mathrm{data}\left[i\right] + 1}{\lambda \left(\lambda - 1\right)} = 0$$

Bayesian Inference

PyMC:

SymPy + RV $\rightarrow$ Theano (array computations) $\rightarrow$ C + CUDA

How do we solve math problems?

```
>>> A = Normal('a', 0, 1)
>>> density(A)
```

$$\frac{\sqrt{2}e^{-\frac{1}{2}z^2}}{2\sqrt{\pi}}$$

```
>>> density(A**2)
```

Use generic transformations taught in Statistics 101, e.g.

$$f_Y(y) = f_X(g^{-1}(y)) \left| \frac{dg^{-1}(y)}{dy} \right|$$

$$\frac{\sqrt{2}e^{-\frac{1}{2}z}\left|\frac{1}{\sqrt{z}}\right|}{2\sqrt{\pi}}$$

How do we solve math problems?

```
>>> A = Normal('a', 0, 1)
>>> B = Normal('b', 0, 1)
>>> density(A**2 + B**2)
```

$$\int_{-\infty}^{\infty} \frac{e^{-\frac{1}{2}(b-a)^2} e^{-\frac{1}{2}z+\frac{1}{2}b^2}}{2\pi|\sqrt{z-b^2}|}\, db$$

How do we solve math problems?

```
>>> A = Normal('a', 0, 1)
>>> B = Normal('b', 0, 1)
>>> density(A**2 + B**2)
```

$$\frac{1}{2}e^{-\frac{1}{2}z}$$

This is a Chi squared distribution with two degrees of freedom

Phenomenological relations:

$$N(0,1)^2 \sim \chi^2(1)$$
$$\chi^2(n) + \chi^2(m) \sim \chi^2(n+m)$$

Term Rewrite System

Rewrite rule:

Source pattern	$tan(x)$
Target pattern	$sin(x)/cos(x)$
Varibles	$x,$

Example:

```
From:   3 + tan(a + b)**2

To:     3 + (sin(a + b) / cos(a + b))**2
```

Term Rewrite System

Rules:

$$tan(a) \rightarrow sin(a)/cos(a)$$
$$sin^2(a) \rightarrow \frac{1 - cos(2a)}{2}$$
$$cos^2(a) \rightarrow \frac{1 + cos(2a)}{2}$$
$$sin(a) + sin(b) \rightarrow 2sin(\frac{a+b}{2})cos(\frac{a+b}{2})$$
$$sin^2(a) + cos^2(a) \rightarrow 1$$
$$sin(a)/cos(a) \rightarrow tan(a)$$
$$\ldots$$

Simplify:

$$sin^2(y) + \frac{sin(z)}{cos(z)} + cos^2(y)$$

Encode Statistical Rewrite Rules

Express patterns:

```
patterns = [
    (Normal(0, 1),                    StandardNormal(),   []),
    (StandardNormal()**2,             ChiSquared(1),      []),
    (ChiSquared(m) + ChiSquared(n),   ChiSquared(n + m),  [n, m]),
    ...
]
```

Define control flow:

```
canonicalize = chain(repeat, bottom_up, choose)
```

Combine:

```
stat_simplify = canonicalize(patterns)
```

Status and Evaluation

- Software:
  - Fully functional
  - Lacks efficient matching for many patterns
  - Maybe integrate into PyMC
- Evaluation:
  - Compare numeric runtimes
  - Compare complexity of problem description

Related Work

- Symbolic Statistics
  - L. Leemis, GD Evans, *APPL: A Probability Programming Language*
  - M. Erwig and S. Kollmansberger *Probabilistic Functional Programming in Haskell*, 2006
- Markov chain Monte Carlo
  - WinBUGS
  - JAGS
  - PyMC
- Term Rewrite Systems - Elan, Maude, Mathematica, Stratego/XT, Coq
- Term Rewrite Systems (CAS)
  - RUBI - AD Rich, DJ Jeffrey *A Knowledge Repository for Indefinite Integration Based on Transformation Rules*
  - H. Fu, X. Zhong, Z. Zeng, *Automated and Readable Simplification of Trigonometric Expressions*

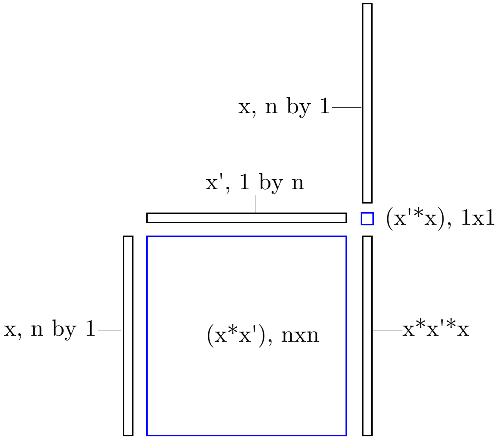
Section 2

Numerical Linear Algebra

The need for a high level array compiler

```
x = ones(10000, 1)

(x*x')*x             Elapsed time is 0.337711 seconds.
x*(x'*x)             Elapsed time is 0.000956 seconds.
```



The need for a high level array compiler

$$\beta = (X^T X)^{-1} X^T y$$

```
beta = (X.T*X).I*X.T*y
```

The need for a high level array compiler

$$\beta = (X^T X)^{-1} X^T y$$

```
beta = solve(X.T*X, X.T*y)
```

The need for a high level array compiler

$$\beta = (X^T X)^{-1} X^T y$$

```
beta = spd_solve(X.T*X, X.T*y)
```

BLAS/LAPACK

Numeric libraries for dense linear algebra

- `DGEMM` - **D**ouble precision **GE**neral **M**atrix **M**ultiply – $\alpha AB + \beta C$

BLAS/LAPACK

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  - `SUBROUTINE DGEMM(TRANSA,TRANSB,M,N,K,ALPHA,A,LDA,B,LDB,BETA,C,LDC)`

BLAS/LAPACK

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BLAS/LAPACK

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- ...
- `DPOSV` - **D**ouble symmetric **PO**sitive definite matrix **S**ol**V**e – $A^{-1}y$

BLAS/LAPACK

Numeric libraries for dense linear algebra

- `DGEMM` - **D**ouble precision **GE**neral **M**atrix **M**ultiply – $\alpha AB + \beta C$
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- ...
- `DPOSV` - **D**ouble symmetric **PO**sitive definite matrix **S**ol**V**e – $A^{-1}y$
  - `SUBROUTINE DPOSV( UPLO, N, NRHS, A, LDA, B, LDB, INFO )`

Necessary Definitions

Language: Multiply, addition, inverse, transpose, trace, determinant, blocks, etc...

```
beta = (X.T*X).I*X.T*y                X.I*X -> Identity
```

Predicates: symmetric, positive_definite, full_rank, orthogonal, lower_triangular, etc....

```
fullrank(X)                           fullrank(X) -> positive_definite(X.T*X)
```

Computations:

```
class SYMM(BLAS):
    inputs    = [alpha, A, B, beta, C]
    outputs   = [alpha*A*B + beta*C]
    condition = symmetric(A) or symmetric(B)
    inplace   = {0: 4} # 0th output stored in 4th input
    template  = ....
```

Mathematical code

Original language definition in Maude

```
eq A (B + C) = (A B) + (A C) .
eq (alpha A)' = alpha A' .
eq A'' = A .
eq inverse(A) A = Identity .
...
eq  X X' is symmetric = True .
ceq X Y  is positive-definite = True  if X is positive-definite
                                     and Y is positive-definite .
ceq X X' is positive-definite = True  if X is full-rank .
```

Eventually moved to SymPy for distribution reasons

Computation

Given:

```
(X.T*X).I*X.T*y
full_rank(X)
```

Produce:

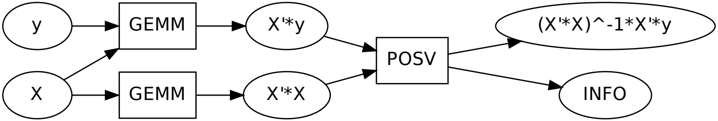
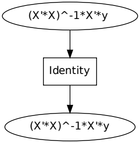
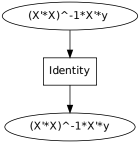


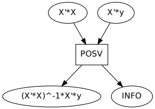
Figure:

Computation

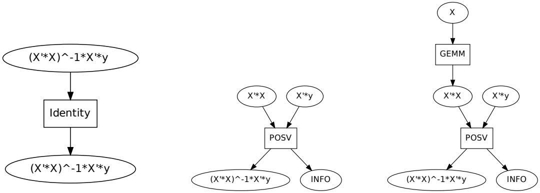


Computation

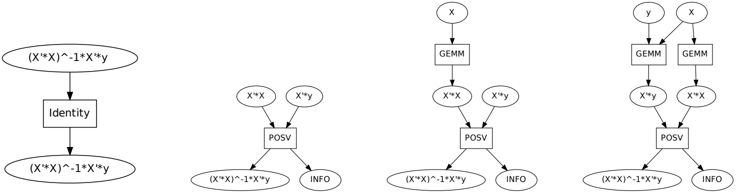




Computation



Computation

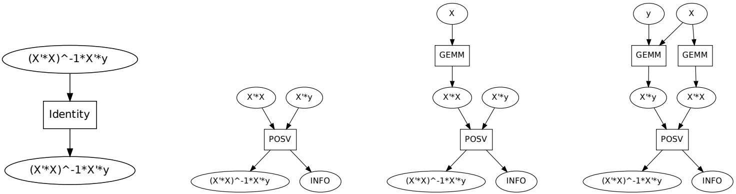


User Experience

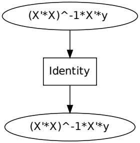
```
X = MatrixSymbol('X', n, m)
y = MatrixSymbol('y', n, 1)

inputs  = [X, y]
outputs = [(X.T*X).I*X.T*y]
facts   = Q.fullrank(X)

f = f2py(next(compile(inputs, outputs, facts)))
```

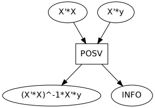
```
subroutine f(X, y, var_7, m, n)
implicit none

integer, intent(in) :: m
integer, intent(in) :: n
real*8, intent(in) :: y(n)            !  y
real*8, intent(in) :: X(n, m)         !  X
real*8, intent(out) :: var_7(m)       !  0, X'*y, (X'*X)^-1*X'*y
real*8 :: var_8(m, m)                 !  0, X'*X
integer :: INFO                       !  INFO

call dgemm('N', 'N', m, 1, n, 1, X, n, y, n, 0, var_7, m)
call dgemm('N', 'N', m, m, n, 1, X, n, X, n, 0, var_8, m)
call dposv('U', m, 1, var_8, m, var_7, m, INFO)

RETURN
END
```

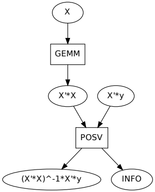
Multiple Results

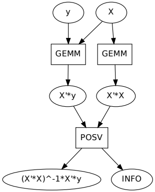


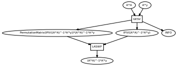
Multiple Results

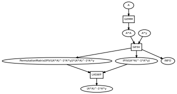


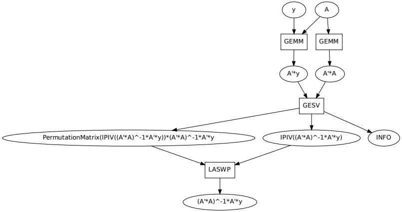












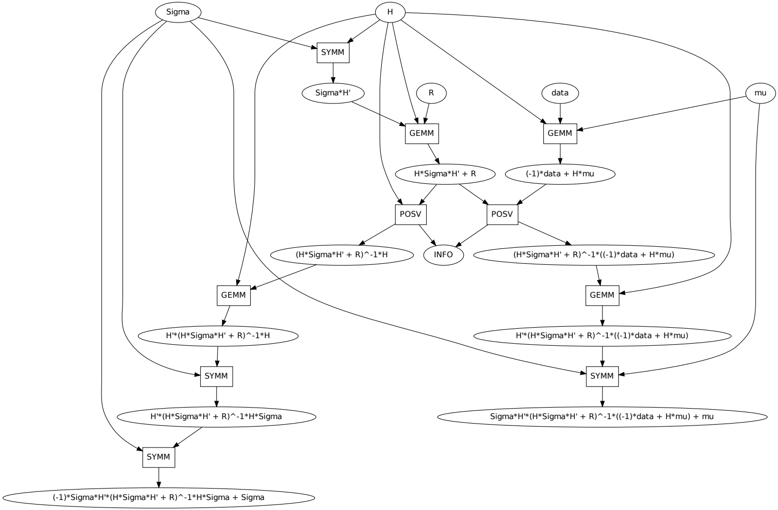
Status and Evaluation

Section 3

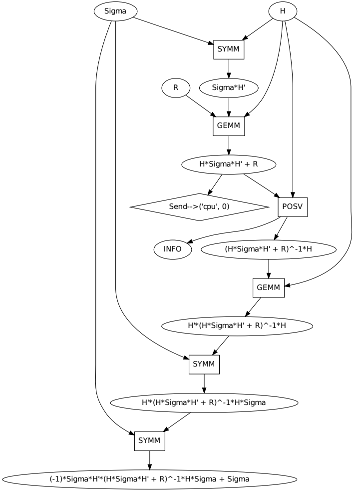
Static Scheduling

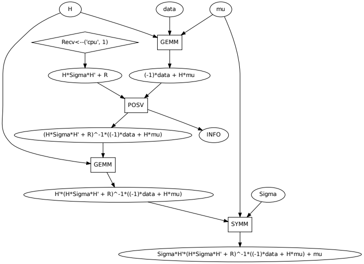
Static Scheduling

```
newmu    = mu + Sigma*H.T * (R + H*Sigma*H.T).I * (H*mu - data)
newSigma = Sigma - Sigma*H.T * (R + H*Sigma*H.T).I * H * Sigma
```



Static Scheduling

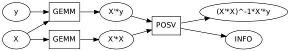




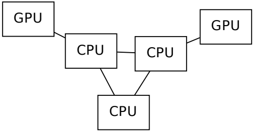
Static Scheduling

Given:

Computation Graph



Worker network



Computation times — task, worker $\rightarrow$ time
Communication times — variable, source, target $\rightarrow$ time

Produce:

Set of computation subgraphs to minimize total runtime

Application - Blocked Cholesky Decomposition

Math Problem:

$$Ax = y \quad \rightarrow \quad LL^T x = y \quad \rightarrow \quad x = L^{-T} L^{-1} y$$

A symmetric positive definite, L lower triangular

$$\begin{bmatrix} A_{11} & A_{21}^T \\ A_{21} & A_{22} \end{bmatrix} = \begin{bmatrix} L_{11} & 0 \\ L_{21} & L_{22} \end{bmatrix} \begin{bmatrix} L_{11} & 0 \\ L_{21} & L_{22} \end{bmatrix}^T$$

$$L_{11} := \text{cholesky}(A_{11})$$

$$L_{21} := A_{21} L_{11}^{-T}$$

$$L_{22} := \text{cholesky}(A_{22} - L_{21} L_{21}^T)$$

Compute Resources:

E.g. Four node system with two GPUs on specific network hardware

Related work

- Performance Modeling
  - E Peise and P Bientinesi. *Performance Modeling for Dense Linear Algebra.* 2012
  - Roman Iakymchuk. *Performance Modeling and Prediction for Linear Algebra Algorithms* 2012
  - JJ Dongarra, RA Vandegeijn, and DW Walker. *Scalability issues affecting the design of a dense linear algebra library* 1994
- Heterogeneous Static Scheduling
  - M. Tompkins. *Optimization Techniques for Task Allocation and Scheduling in Distributed Multi-Agent Operations.* 2003
  - H. Topcuoglu, S. Hariri, M. Wu. *Performance-effective and low-complexity task scheduling for heterogeneous computing.* 2002
  - Suggestions?
- Automated Dense Linear Algebra
  - ScaLAPACK, PlaLAPACK, BLACS
  - FLAME - Language for blocked matrix algorithms
    - SuperMatrix - Dynamic shared memory variant
    - Elemental - Distributed memory variant
  - Magma - Hybrid LAPACK
  - Spiral - Hardware specific numeric code generation with internal computation language

Status and Evaluation

- Have done - Software
  - Implemented Schedulers
  - Implemented rudimentary cost model
  - Everything hooks up well
- Will do - Compare existing schedulers with
  - Schedulers: IP, Heuristic, Naive dynamic scheduling
  - Variety of block / problem sizes
  - Variety of desired algorithms
  - Variety of timing models
  - Compare scheduling times vs execution times
- Could do -
  - Implement direct cost model (run and profile each task)
  - Comparison against FLAME/Magma

DAG Ordering

Recv and Send return control immediately.

RecvWait and SendWait block until communication terminates.

A, B, C, D are computation tasks

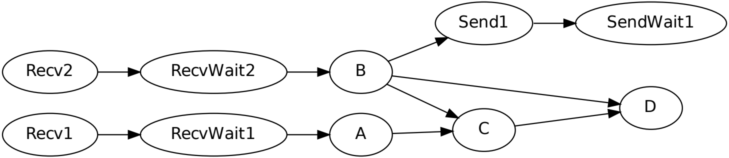


Figure:

```
Order 1: R1 RW1 R2 RW2 A B C D S1 SW1

Order 2: R2 R1 RW2 B S1 RW1 A C D SW1
```

DAG Ordering

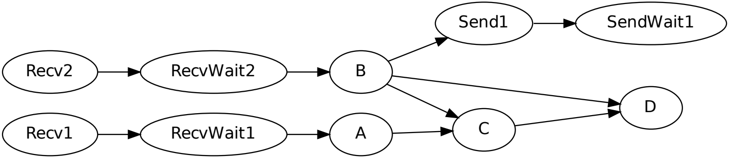
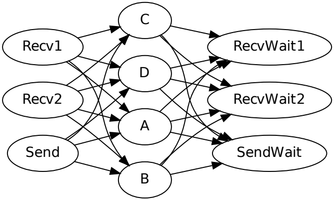


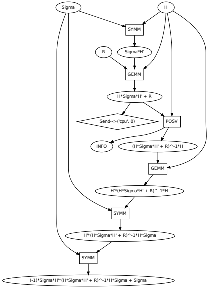
Figure:

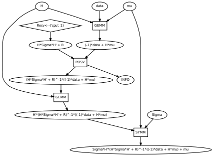


DAG Ordering

```
def dependence(a, b):
    if depends((a, b)): return  1
    if depends((b, a)): return -1
    return 0

def mpi_send_wait_key(a):
    """ Wait as long as possible on Waits, Start Send/Recvs early """
    if isinstance(a.op, (MPIRecvWait, MPISendWait)):       return 1
    if isinstance(a.op, (MPIRecv, MPISend)):               return -1
    return 0

def mpi_tag_key(a):
    """ Break MPI ties by using the variable tag - prefer lower tags first """
    if isinstance(a.op, (MPISend, MPIRecv, MPIRecvWait, MPISendWait)):
        return a.op.tag
    return 0
```

Thank You





Slides: http://github.com/mrocklin/candidacy-exam/

Section 4

Extras

Inplace

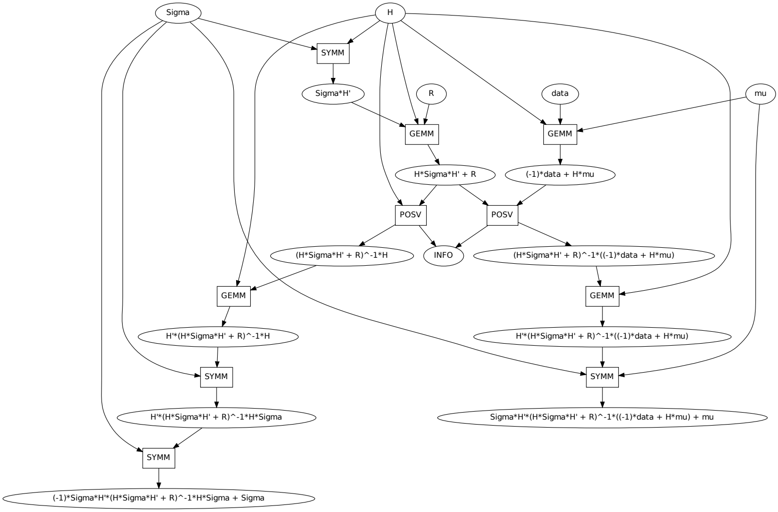


Figure:

Inplace

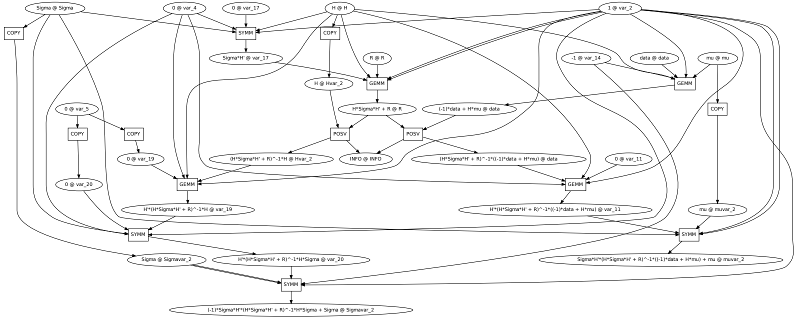


Figure: