Deriving Efficient Parallel Implementations of Algorithms Operating on General Sparse Matrices using Program Transformation

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Clarity V Efficiency

High-level, architecture-independent programs

- Easier to construct
- Easier to understand
- Portable

Efficient programs

- Tailored to particular machine: non-portable
- Awash with details
- Difficult to construct
- Difficult to understand

Example: Transpose of a Matrix

Definition: transpose A^T of $m \times n$ matrix A is an $n \times m$ matrix such that

$$\forall i, j : A^T[i, j] \equiv A[j, i]$$

High-level implementation

```
function transpose(A,m,n)
  = generate([n,m],fn(i,j)=>A[j,i])
```

Efficient sequential implementation for square matrix (m=n)

```
SUBROUTINE transpose(A,n)
DO i=1,n
  DO j=i+1,n
    t := A[i,j]
    A[i,j] := A[j,i]
    A[j,i] := t
  END
END
```

Our resolution

Programmer constructs specification; implementation *automatically* derived.

Specification language

Functional programming language

- Mathematically based
- Simple semantics: easily understood
- Useful mathematical properties
- Executable prototypes

Implementation language

Whatever required by implementation environment; usually version of Fortran or C.

- Efficient
- Good vendor support
- More convenient than machine language

Derivation by program transformation

Program Transformations

Program rewrite rules:

$$pattern \rightarrow replacement$$

All occurrences of $pattern$ in program changed to $replacement$.

- Achieves a small, local change
- Based on formal properties
  Clearly preserves meaning of program
- Formally defined in wide spectrum grammar
- Formal proof possible

Derivations

Sequences of transformations

- Complete metamorphosis through many applications of many transformations
- Automatically applied by TAMPR system

Family of Derivations

Derivation performed in steps

- *Sub-derivations*
- *Intermediate forms* between specification and implementation languages

For example:

$$\text{SML} \longrightarrow \lambda\text{-calculus} \longrightarrow \text{Fortran77}$$

Same intermediate form for:

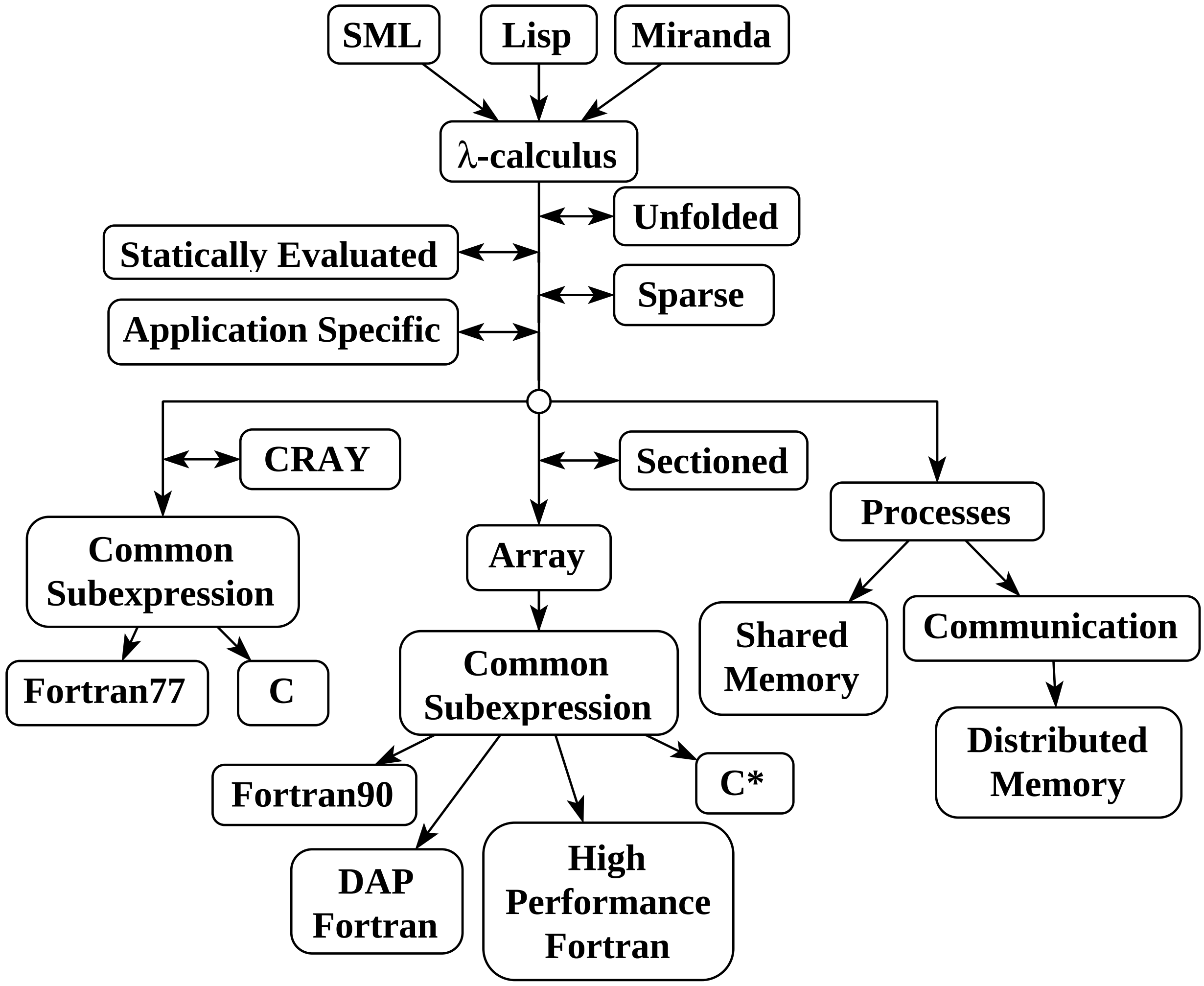
- other specification languages
- other architectures/implementation languages

Combinations have included:

$$\left.\begin{array}{c}\text{SML}\\ \text{Lisp}\\ \text{Miranda}\end{array}\right\} \longrightarrow \lambda\text{-calculus} \longrightarrow \left\{\begin{array}{c}\text{Fortran}\\ \text{CRAY Fortran}\\ \text{DAP Fortran}\\ \text{C}\end{array}\right.$$

Other sub-derivations/intermediate forms for:

- Optimization e.g.
  function unfolding
  common subexpression elimination
- Tailoring for particular forms of data
  e.g. sparse matrices



Sparse Matrices

We consider a matrix which has a fixed number of non-zero elements per row:

$$\begin{array}{ccccc} \text{Sparse matrix} & & \text{Primary} & & \text{Secondary} \\ \begin{bmatrix} 0 & 1 & 0 & 0 & 2 \\ 3 & 0 & 0 & 0 & 0 \\ 0 & 4 & 5 & 0 & 0 \\ 0 & 0 & 0 & 6 & 7 \\ 8 & 0 & 9 & 0 & 0 \end{bmatrix} & \longrightarrow & \begin{bmatrix} 1 & 2 \\ 3 & 0 \\ 4 & 5 \\ 6 & 7 \\ 8 & 9 \end{bmatrix} & & \begin{bmatrix} 2 & 5 \\ 1 & 2 \\ 2 & 3 \\ 4 & 5 \\ 1 & 3 \end{bmatrix} \end{array}$$

$$A_p[i,j'] \equiv A[i, [A_s[i,j']]] \quad .$$

- This form of sparsity is efficient in storage if the number of non-zeros averaged over the rows is not much less than the maximum number of non-zeros.
- This is an example of a particular form of sparsity.
  - An illustration where tailoring for a compressed data representation and a parallel computer is performed.
  - Other representations are possible by substituting the mapping phase of the transformations (later).

Example

Matrix-vector multiplication

$$\begin{bmatrix} \cdots \\ \cdots \\ \hline 1 \quad 2 \quad 3 \quad 4 \\ \hline \cdots \\ \cdots \\ \cdots \end{bmatrix} \times \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} = \begin{bmatrix} \cdots \\ \cdots \\ \hline 1a + 2b + 3c + 4d \\ \hline \cdots \\ \cdots \\ \cdots \end{bmatrix}$$

```
fun times(U:vector,V:vector):vector
  = generate(size(U),fn(i:int)=>U@[i]*V@[i])
fun sum(U:vector):real
  = reduce(U,+,0.0)
fun innerproduct(U:vector,V:vector):real
  = sum(times(U,V))

fun mvmult(A:matrix,V:vector):vector
  = generate(size(A,0),
     fn(i:int)=>innerproduct(row(A,i),V))
```

SML specification

Data parallel functions

- `generate` defines vector/matrix
- `reduce` combines elements of vector/matrix into single value

Derivation Stages

1. Abstract Functional Specification

```
fun times:real vector × real vector → real vector
 = λ.U,V.generate(size(U),
    λ.i.real.times(element(U,i),element(V,i)))

fun sum:real vector → real
 = λ.V.reduce(+,0.0,size(V),λ.i.element(V,i))

fun innerproduct:real vector × real vector → real
 = λ.U,V.sum(times(U,V))

fun mvmult:real matrix × real vector → real vector
 = λ.M,V.generate(size(M,0),
   λ.i.innerproduct(row(M,i),V))
```

2. Unfolding and Static Evaluation

```
fun mvmult = generate(n,
  λ.i.reduce(+,0.0,n,
    λ.j.times(element(A,[i,j]),element(V,[j]))))
```

where we assume that the sizes of A and V have been defined in terms of some parameter **n** .

Derivation Stages - Continued

3. Sparse Specialization

Phase 1:annotation

Explicitly distinguish non-zero elements from zero elements.

```
fun mvmult = generate(n,
  λ.i.reduce(+,0.0,n,
    λ.j.times(
      if ([i,j] ∈ fixed_row_number([n,n],w))
      then element(A,[i,j])
      else 0.0,
      element(V,[j]))))
```

`fixed_row_number` is the set of significant indices of the matrix.

Derivation Stages - Continued

3. Sparse Specialization

Phase 2: optimization

$\longrightarrow$

```
fun mvmult = generate(n,
  λ.i.reduce(+,0.0,n,
    λ.j.if ([i,j] ∈ fixed_row_number([n,n],w))
    then times(element(A,[i,j]),element(V,[j]))
    else 0.0))
```

$\longrightarrow$

```
fun mvmult = generate(n,
  λ.i.reduce(+,0.0,
    row(fixed_row_number([n,n],w),i),
    λ.j.times(element(A,[i,j]),element(V,[j]))))
```

Function **row** returns the set of indices of non-zero elements in a specified row.

Derivation - Continued

3. Sparse Specialization

Phase 3: mapping

Provide a compact realization for sparse matrices.

$$[i,j] \rightarrow [i, locate(shape, [i,j]\,)\,]$$

and the inverse

$$[i,j'] \rightarrow [i, secondary(\,[i,j']\,)\,] \quad .$$

```
fun mvmult = generate(n,
  λ.i.reduce(+,0.0,w,
    λ.j′.times(
      element(A:[i,j′]),
      element(V,[secondary(A,[i,j′])]))))
```

Derivation - Continued

4. Imperative Implementation

```
      integer n,w
      parameter(n=??,w=???)
      real Ap(n,w),U(n),V(n)
      integer As(n,w)
      integer i,j

      do 100 i=1,n
      U(i)=0.0
      do 101 j=1,w
      U(i)=U(i)+Ap(i,j)*V(As(i,j))
101   continue
100   continue
      end
```

Conjugate Gradient Definition

To solve Ax=b, where A is a positive definite symmetric $n \times n$ matri x:

Set an initial approximation vector x_0,

calculate the initial residual r_0=$b - Ax_0$,

set the initial search direction p_0=r_0;

then, for i=$0, 1, \ldots,$

(a) calculate the coefficient α_i=$p_i^T r_i / p_i^T A p_i$,

(b) set the new estimate x_{i+1}=x_i + $\alpha_i p_i$,

(c) evaluate the new residual r_{i+1}=$r_i - \alpha_i A p_i$,

(d) calculate the coefficient β_i=$-r_{i+1} A p_i / p_i^T A p_i$,

(e) determine the new direction p_{i+1}=r_{i+1} + $b_i p_i$,

continue until either r_i or p_i is zero.

from Modi,p152

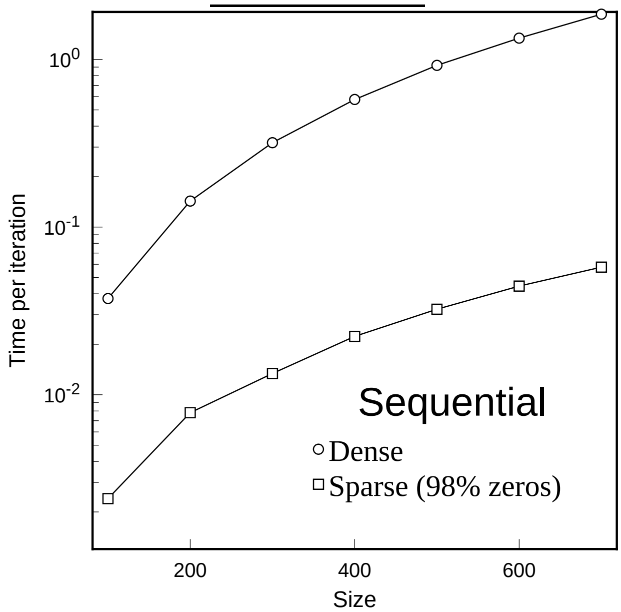
Conjugate Gradient Specification

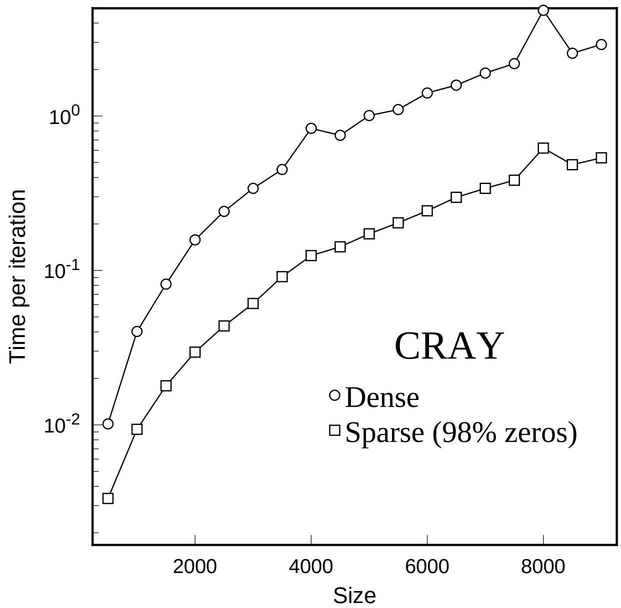
```
val epsilon:real = 1.0E-14;
type cgstate
 = real vector*real vector*real vector*real vector*int;

fun cg_construct(A:real matrix,b:real vector):cgstate
 = let
  val x0:real vector = constant(shape(b),0.0);
  val r0:real vector = b;
  val p0:real vector = r0;
  val q0:real vector = A*p0;

  fun is_accurate_solution((x,r,p,q,cnt):cgstate):bool
   = innerproduct(r,r)<epsilon;


  fun cg_iteration((x,r,p,q,cnt):cgstate):cgstate
   =  let
    val rr:real = innerproduct(r,r);
    val cnt′:int = cnt+1;
    val alpha:real = rr/innerproduct(q,q);
    val x′:real vector = x+p*alpha;
    val r′:real vector = r-transpose(A)*q*alpha;
    val beta:real = innerproduct(r′,r′)/rr;
    val p′:real vector = r′+p*beta;
    val q′:real vector = A*r′+q*beta
  in
    cgstate(x′,r′,p′,q′,cnt′)
  end


in
  iterate(cg_iteration,
    cgstate(x0,r0,p0,q0,0),
    is_accurate_solution)
end
```

Conjugate Gradient - Derived

```
      integer n,w
      parameter(n=SIZE,w=2*n/100)
      real x(n), q(n), p(n), b(n)
      integer cnt, k, As(n,w), i, j
      real Ap(n,w), r(n), r1(n), alpha, atq(n), beta, g63, rr
  200 continue
      rr = 0.0
      do 210 j = 1,n,1
      rr = rr+r(j)*r(j)
  210 continue
      if (sqrt (rr) .lt.1E-14) then
      goto 500
      else
      alpha = 0.0
      do 220 i = 1,n,1
      alpha = alpha+q(i)*q(i)
  220 continue
      alpha = rr/alpha
      do 230 i = 1,n,1
      atq(i) = 0.0
  230 continue
      do 240 i = 1,n,1
      do 240 k = 1,w,1
      atq(As(i,k)) = atq(As(i,k))+Ap(i,k)*q(i)
  240 continue
      do 260 j=1,n
      r1(j) = r(j)-atq(j)*alpha
  260 continue
      beta = 0.0
      do 270 j = 1,n,1
      beta = beta+r1(j)*r1(j)
  270 continue
      beta = beta/rr
      cnt = cnt+1
      do 280 j = 1,n,1
      x(j) = x(j)+p(j)*alpha
  280 continue
      do 290 j = 1,n,1
      p(j) = r1(j)+p(j)*beta
  290 continue
      do 300 i=1,n,1
      r(i) = r1(i)
  300 continue
      do 340 j = 1,n,1
      g63 = 0.0
      do 330 k = 1,w,1
      g63 = g63+Ap(j,k)*r1(As(j,k))
  330 continue
      q(j) = g63+q(j)*beta
  340 continue
      goto 200
      endif
  500 continue
      end
```

Results





Conjugate Gradient

Assessment

Techniques have been applied to significant algorithms for sequential,vector, array and shared-memory architectures.

Comparing with independent, manually constructed implementations:

- Derived implementations similar.
- Execution performance equal or better.

Techniques are being extended for yet more complex algorithms, for distributed and shared memory parallel architectures and for further special data structures.

Conclusion-Summary

With derivational approach, programmer

- develops implementation techniques
- encodes techniques as derivations

Reusability
Multiple specifications
Multiple implementations of each
Algorithm modified: modify specification
and re-apply derivation

- it is possible to experiment with different implementations easily.

Extensibility
New optimization technique
or new architecture
or new data representation:
'slot in' new sub-derivation

Transferability
Sub-derivation requires no expertise to use
One programmer may use another's work

Correctness
Correctness of transformations
implies correctness of implementation