

# Title Text

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## Abstract

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## 1. Introduction

Computing with arrays has been a constantly important paradigm in the history of computing. For this reason we have seen a plethora of formalisms and languages being developed to aid theoreticians and developers to produce more suitable abstractions and faster programs. Examples include Fortran, APL and Matlab but the list goes on and on. Having many different options to choose from can be a good thing but it can also lead to a balkanization of the community. When researchers dedicated to different formalisms can no longer talk to each other, it inhibits collaborations and limits the impact of innovation.

In this paper we aim to rectify some of the fragmentation of the high-performance array programming community by relating two particular formalisms: Mathematics of Arrays and Pull arrays. On the surface they appear rather different but at their core they share many principles and properties which we will examine in this paper. In particular we will highlight the following points:

- We give an introduction to both MoA (section 2) and Pull arrays (section 3).
- The two formalisms are compared with respect to types (section 4.1), fusion/ $\psi$ -reduction (section 4.2), how they deal with higher dimensions (section 4.3) and notation (section 4.4).

We would like to stress that we are not looking to declare a winner. Instead our intention is that this paper can serve as a help for the two communities to be able to learn about each others work.

## 2. Overview of MoA

MoA, an acronym for *A Mathematics of Arrays*[1], is a theory of arrays with both an algebra and a calculus of indexing based on shapes, i.e. sizes of each dimension. The index calculus, referred to as *The Psi Calculus*, gets its names from the *Psi* function which is the foundational function in the theory. The name *Psi* was inspired by Dirac's *Psi Vectors* and his communications with Einstein to have a mathematical way to reason about them. These results began with the awareness that Iverson's APL[20] was inspired by Sylvester's Universal Algebra[44] and the fact that he and Cayley invented matrices. The programming language, APL, embodied Ken's notation into an interpretive computing environment. It was at this point that theoretical anomalies were introduced.

Not only did Ken believe that APL's array algebra was the ideal basis for a programming language, he (and others) believed that an ideal machine language supported array operations. This led to HP building an APL machine based on Phil Abram's dissertation[2]. Abrams was the first to identify ways to define an algebra of arrays based on shapes; others attempted to put closure on his work[15, 17]. Abrams believed that if array operations were based on indexing with shapes, all indexing in the array expression could be composed and thus could minimize the creation (and deletion) of temporary arrays, a huge overhead. One of the reasons HP's APL Machine did not succeed was that this analysis was done at run time. It was Alan Perlis, and later others[8, 27], who realized that these optimizations should be done at compile time. Attempts at compilation led Perlis to realize that anomalies in the language [13] made it difficult to optimize and impossible to verify correctness of programs leading him to recommend a functional array calculator based on the lambda calculus[45, 46]. This awareness led to Mullin's collaborations with Klaus Berkling to combine MoA, Psi Calculus, and the Lambda Calculus, theoretically an ideal environment[6] and basis for a functional programming language with arrays[7, 16, 28, 31, 32, 35].

MoA and the Psi Calculus, as a theory, have also been used to describe and verify hardware[37, 40, 41], describe the partitioning and scheduling of array operations (and their costs)[10, 12, 26, 30, 33, 38, 39], and the formulation of parallel and distributed processing[36]. MoA and  $\psi$ -Calculus, can be used to abstract complex processor memory layouts for tensor/array expressions, reduce these expressions first to a semantic normal form (Denotational Normal Form-DNF) then to an Operational Normal Form (ONF). The ONF describes how to *build* the code using *start*, *stop*, *stride*, and *count*: a universal machine abstraction. This is possible by *abstractly* lifting the dimension of an expression to include all aspects of a processor, memory, communication topology. For example, to map a 2-d array expression to  $n$  processors we would lift the dimension to 3-d.

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## Elements of the theory

### Indexing and Shapes

The central operation of MoA is the indexing function

$$p\psi A$$

in which a vector of  $n$  integers  $p$  is used to select an item of the  $n$ -dimensional array  $A$ . The operation is generalized to select a partition of  $A$ , so that if  $q$  has only  $k < n$  components then

$$q\psi A$$

is an array of dimensionality  $n - k$  and  $q$  selects among the possible choices for the first  $k$  axes. In MoA zero origin indexing is assumed. For example, if  $A$  is the 3 by 5 by 4 array

$$\begin{bmatrix} 0 & 1 & 2 & 3 \\ 4 & 5 & 6 & 7 \\ 8 & 9 & 10 & 11 \\ 12 & 13 & 14 & 15 \\ 16 & 17 & 18 & 19 \end{bmatrix} \begin{bmatrix} 20 & 21 & 22 & 23 \\ 24 & 25 & 26 & 27 \\ 28 & 29 & 30 & 31 \\ 32 & 33 & 34 & 35 \\ 36 & 37 & 38 & 39 \end{bmatrix} \begin{bmatrix} 40 & 41 & 42 & 43 \\ 44 & 45 & 46 & 47 \\ 48 & 49 & 50 & 51 \\ 52 & 53 & 54 & 55 \\ 56 & 57 & 58 & 59 \end{bmatrix}$$

then

$$< 1 > \psi A = \begin{bmatrix} 20 & 21 & 22 & 23 \\ 24 & 25 & 26 & 27 \\ 28 & 29 & 30 & 31 \\ 32 & 33 & 34 & 35 \\ 36 & 37 & 38 & 39 \end{bmatrix}$$

$$< 2 \ 1 > \psi A = < 44 \ 45 \ 46 \ 47 >$$

$$< 2 \ 1 \ 3 > \psi A = 47$$

Most of the common array manipulation operations found in languages like Fortran90, Matlab, ZPL, etc., can be defined from  $\psi$  and a few elementary vector operations.

We now introduce notation to permit us to define  $\psi$  formally and to develop the *Psi Correspondence Theorem* [29], which is central to the effective exploitation of MoA in array computations. We will use  $A, B, \dots$  to denote an array of numbers (integer, real, or complex). An array's dimensionality will be denoted by  $d_A$  and will be assumed to be  $n$  if not specified.

The shape of an array  $A$ , denoted by  $s_A$ , is a vector of integers of length  $d_A$ , each item giving the length of the corresponding axis. The total number of items in an array, denoted by  $t_A$ , is equal to the product of the items of the shape. The subscripts will be omitted in contexts where the meaning is obvious.

A full index is a vector of  $n$  integers that describes one position in an  $n$ -dimensional array. Each item of a full index for  $A$  is less than the corresponding item of  $s_A$ . There are precisely  $t_A$  indices for an array (due to a zero index origin). A partial index of  $A$  is a vector of  $0 \leq k < n$  integers with each item less than the corresponding item of  $s_A$ .

We will use a tuple notation (omitting commas) to describe vectors of a fixed length. For example,

$$< i \ j \ k >$$

denotes a vector of length three.  $<>$  will denote the empty vector which is also sometimes written as  $\Theta$ .

For every  $n$ -dimensional array  $A$ , there is a vector of the items of  $A$ , which we denote by the corresponding lower case letter, here  $a$ . The length of the vector of items is  $t_A$ . A vector is itself a one-dimensional array, whose shape is the one-item vector holding the length. Thus, for  $a$ , the vector of items of  $A$ , the shape of  $a$  is

$$s_a = < t_A >$$

and the number of items or total number of components  $a^1$  is

$$t_a = t_A.$$

The precise mapping of  $A$  to  $a$  is determined by a one-to-one ordering function, *gamma*. Although the choice of ordering is arbitrary, it is essential in the following that a specific one be assumed. By convention we assume the items of  $A$  are placed in  $a$  according to the lexicographic ordering of the indices of  $A$ . This is often referred to as *row major ordering*. Many programming languages lay out the items of multidimensional arrays in memory in a contiguous segment using this ordering. Fortran uses the ordering corresponding to a transposed array in which the axes are reversed *column major*. Scalars are introduced as arrays with an empty shape vector.

There are two equivalent ways of describing an array  $A$ :

- (1) by its shape and the vector of items, i.e.  $A = \{s_A, a\}$ , or
- (2) by its shape and a function that defines the value at every index  $p$ .

These two forms have been shown to be formally equivalent [18]. We wish to use the second form in defining functions on multidimensional arrays using their Cartesian coordinates (indices). The first form is used in describing address manipulations to achieve effective computation.

To complete our notational conventions, we assume that  $p, q, \dots$  will be used to denote indices or partial indices and that  $u, v, \dots$  will be used to denote arbitrary vectors of integers. In order to describe the  $i_{th}$  item of a vector  $a$ , either  $a_i$  or  $a[i]$  will be used. If  $u$  is a vector of  $k$  integers all less than  $t_A$ , then  $a[u]$  will denote the vector of length  $k$ , whose items are the items of  $a$  at positions  $u_j$ ,  $j = 0, \dots, k - 1$ .

Before presenting the formal definition of the  $\psi$  indexing function we define a few functions on vectors:

$u \ ++ \ v$	catentation of vectors $u$ and $v$
$u \ + \ v$	itemwise vector addition assuming $t_u = t_v$
$u \ \times \ v$	itemwise vector multiplication
$n \ + \ u, u \ + \ n$	addition of a scalar to each item of a vector
$n \ \times \ u, u \ \times \ n$	multiplication of each item of a vector by a scalar
$\iota \ n$	the vector of the first $n$ integers starting from 0
$\pi \ v$	a scalar which is the product of the components of $v$
$k \ \Delta \ u$	when $k \geq 0$ the vector of the first $k$ items of $u$ , (called <i>take</i> ) and when $k < 0$ the vector of the last $k$ items of $u$
$k \ \nabla \ u$	when $k \geq 0$ the vector of $t_u - k$ last items of $u$ , (called <i>drop</i> ) and when $k < 0$ the vector of the first $t_u -  k $ items of $u$
$k \ \theta \ u$	when $k \geq 0$ the vector of $(k \ \nabla \ u) \ ++ (k \ \Delta \ u)$ and when $k < 0$ the vector of $(k \ \Delta \ u) \ ++ (k \ \nabla \ u)$

**DEFINITION 1.** Let  $A$  be an  $n$ -dimensional array and  $p$  a vector of integers. If  $p$  is an index of  $A$ ,

$$p\psi A = a[\gamma(s_A, p)],$$

where

$$\begin{aligned} \gamma(s_A, p) &= x_{n-1} \quad \text{defined by the recurrence} \\ x_0 &= p_0, \\ x_j &= x_{j-1} * s_j + p_j, \quad j = 1, \dots, n-1. \end{aligned}$$

If  $p$  is partial index of length  $k < n$ ,

$$p\psi A = B$$

where the shape of  $B$  is

$$s_B = k \ \nabla \ s_A,$$

<sup>1</sup> We also use  $\tau a$ ,  $\delta a$ , and  $\rho a$  to denote total number of components, dimensionality and shape of  $a$ .

and for every index  $q$  of  $B$ ,

$$q\psi B = (p ++ q)\psi A$$

The definition uses the second form of specifying an array to define the result of a partial index. For the index case, the function  $\gamma(s, p)$  is used to convert an index  $p$  to an integer giving the location of the corresponding item in the row major order list of items of an array of shape  $s$ . The recurrence computation for  $\gamma$  is the one used in most compilers for converting an index to a memory address [22].

COROLLARY 1.  $\langle \rangle \psi A = A$ .

The following theorem shows that a  $\psi$  selection with a partial index can be expressed as a composition of  $\psi$  selections.

THEOREM 1. Let  $A$  be an  $n$ -dimensional array and  $p$  a partial index so that  $p = q ++ r$ . Then

$$p\psi A = r\psi(q\psi A).$$

*Proof:* The proof is a consequence of the fact that for vectors  $u, v, w$

$$(u ++ v) ++ w = u ++ (v ++ w).$$

If we extend  $p$  to a full index by  $p ++ p'$ , then

$$\begin{aligned} p'\psi(p\psi A) &= (p ++ p')\psi A \\ &= ((q ++ r) ++ p')\psi A \\ &= (q ++ (r ++ p'))\psi A \\ &= (r ++ p')\psi(q\psi A) \\ &= p'\psi(r\psi(q\psi A)) \\ p\psi A &= r\psi(q\psi A) \end{aligned}$$

which completes the proof.

We can now use  $\psi$  to define other operations on arrays. For example, consider definitions of *take* and *drop* for multidimensional arrays.

DEFINITION 2 (take:  $\Delta$ ). Let  $A$  be an  $n$ -dimensional array, and  $k$  a non-negative integer such that  $0 \leq k < s_0$ . Then

$$k \Delta A = B$$

where

$$s_B = \langle k \rangle ++ (1 \nabla s_A)$$

and for every index  $p$  of  $B$ ,

$$p\psi B = p\psi A.$$

(In MoA  $\Delta$  is also defined for negative integers and is generalized to any vector  $u$  with its absolute value vector a partial index of  $A$ . The details are omitted here.)

DEFINITION 3 (reverse:  $\Phi$ ). Let  $A$  be an  $n$ -dimensional array. Then

$$s_{\Phi A} = s_A$$

and for every integer  $i$ ,  $0 \leq i < s_0$ ,

$$\langle i \rangle \psi \Phi A = \langle s_0 - i - 1 \rangle \psi A.$$

This definition of  $\Phi$  does a reversal of the 0th axis of  $A$ .

Note also that all operations are over the 0th axis. The operator  $\Omega$  [34] extends operations over all other dimensions.

### Example

Consider the evaluation of the following expression using the 3 by 5 by 4 array,  $A$ , introduced in Section 2.

$$\langle 1 \ 2 \rangle \psi (2 \Delta \Phi A) \quad (1)$$

where  $A$  is the array given in the previous section. The shape of the result is

$$\begin{aligned} & 2 \nabla s_{(2 \Delta \Phi A)} \\ &= 2 \nabla (\langle 2 \rangle ++ (1 \nabla s_{\Phi A})) \\ &= 2 \nabla (\langle 2 \rangle ++ (1 \nabla s_A)) \\ &= 2 \nabla (\langle 2 \rangle ++ \langle 5 \ 4 \rangle) \\ &= 2 \nabla \langle 2 \ 5 \ 4 \rangle \\ &= \langle 4 \rangle. \end{aligned} \quad (2)$$

The expression can be simplified using the definitions:

$$\begin{aligned} & \langle 1 \ 2 \rangle \psi (2 \Delta \Phi A) \\ &= \langle 1 \ 2 \rangle \psi \Phi A \\ &= \langle 2 \rangle \psi (\langle 1 \rangle \psi \Phi A) \\ &= \langle 2 \rangle \psi (\langle 3 - 1 - 1 \rangle \psi A) \\ &= \langle 1 \ 2 \rangle \psi A \end{aligned} \quad (3)$$

This process of simplifying the expression for the item in terms of its Cartesian coordinates is called *Psi Reduction*. The operations of MoA have been designed so that all expressions can be reduced to a minimal normal form [34]. Some MoA operations defined by  $\psi$  are found in Fig.1.

Symbol	Name	Description
$\delta$	Dimensionality	Returns the number of dimensions of an array.
$\rho$	Shape	Returns a vector of the upper bounds or sizes of each dimension in an array.
$\iota \xi^n$	Iota	When $n = 0$ (scalar), returns a vector containing elements 0, to $\xi^0 - 1$ . When $n = 1$ (vector), returns an array of indices defined by the shape vector $\xi^1$
$\psi$	Psi	The main indexing function of the Psi Calculus which defines all operations in MoA. Returns a scalar if a full index is provided, a sub-array otherwise.
rav	Ravel	vectorizes a multi-dimensional array based on an array's layout( $\gamma_{row}, \gamma_{col}, \gamma_{sparse}, \dots$ )
$\gamma$	Gamma	Translates indices into offsets given a shape.
$\gamma'$	Gamma Inverse	Translates offsets into indices given a shape.
$\hat{s} \hat{\rho} \xi$	Reshape	Changes the shape vector of an array, possibly affecting its dimensionality. Reshape depends on layout( $\gamma$ ).
$\pi \vec{x}$	Pi	Returns a scalar and is equivalent to $\prod_{i=0}^{(\tau x)-1} x[i]$
$\tau$	Tau	Returns the number of components in an array, ( $\tau \xi \equiv \pi(\rho \xi)$ )
$\xi_l ++ \xi_r$	Catenate	Concatenates two arrays over their primary axis.
$\xi_l f \xi_r$	Point-wise Extension	A data parallel application of $f$ is performed between all elements of the arrays.
$\sigma f \xi_r$	Scalar Extension	$\sigma$ is used with every component of $\xi_r$ in the data parallel application of $f$ .
$\xi_l f \sigma$		
$\Delta$	Take	Returns a sub-array from the beginning or end of an array based on its argument being positive or negative.
$\nabla$	Drop	The inverse of Take
$op_{red}$	Reduce	Reduce an array's dimension by one by applying $op$ over the primary axis of an array.
$\Phi$	Reverse	Reverses the components of an array.
$\Theta$	Rotate	Rotates, or shifts cyclically, components of an array.
$\nabla$	Transpose	Transposes the elements of an array based on a given permutation vector
$\Omega$	Omega	Applies a unary or binary function to array argument(s) given partitioning information. $\Omega$ is used to perform all operations (defined over the primary axis only) over all dimensions.

Figure 1. Summary of MoA Operations

### Higher Order Operations

Thus far operation on arrays, such as concatenation, rotation, etc., have been performed over their 0th dimensions. We introduce the higher order binary operation  $\Omega$ , which is defined when its left

```

-- Mapping a function over an array
map :: (a -> b) -> Pull a -> Pull b
map f (Pull ixf l) = Pull (f . ixf) l

-- Apply a binary operation itemwise on two arrays
zipWith :: (a -> b -> c)
        -> Pull a -> Pull b -> Pull c
zipWith f (Pull ixf1 l1) (Pull ixf2 l2)
    = Pull (\i -> f (ixf1 i) (ixf2 i)) (min l1 l2)

-- Takes the n first elements of an array
take :: Int -> Pull a -> Pull a
take n (Pull ixf l) = Pull ixf (min n l)

-- Drops the n first elements of an array
drop :: Int -> Pull a -> Pull a
drop n (Pull ixf l)
    = Pull (\i -> ixf (i + n)) (max (l - n) 0)

-- Rotate an array k steps to the left
rotate :: Int -> Pull a -> Pull a
rotate k (Pull ixf l)
    = Pull (\i -> ixf ((i + k) `mod` l)) l

```

**Figure 2.** Example functions on pull arrays

argument is a unary or binary operation and its right argument is a vector describing the dimension upon which operations are to be performed, or which sub-arrays are used in operations. The dimension upon which operations are to be performed is often called the *axis* of operation. The result of  $\Omega$  is a unary or binary operation.

### 3. Overview of Pull arrays

The functional programming community has recently gained an increased interest in high performance parallel array programming [3, 5, 9, 21, 23, 24, 43]. One of the central abstractions in this line of work is the *pull array*, also known as delayed array. The can be defined as follows (we use Haskell [25] to demonstrate functions programs).

```

data Pull a = Pull { ixf      :: (Int -> a)
                    , length :: Int
                    }

```

Arrays are represented as functions from index to element. We refer to this function as an *index function*. Additionally arrays also have a length.

This representation has several advantages:

- *Parallelism*. Since each element is computed independently, they can easily be computed in parallel.
- *Fusion*. When functions on pull arrays are composed, the intermediate arrays can be automatically removed.
- *Compositionality*. Pull arrays provide a wealth of compositional and highly reusable combinators. These can be composed together to write high-level programs which typically are easier to understand than monolithic array processing code.

#### 3.1 Fusion

As mentioned, one of the most important advantages of Pull arrays is that they support fusion[4, 14, 21]. Fusion is a program transformation which removes intermediate data structures and is a decendant of deforestation [47]. Fusion supersedes transformations such

as loop fusion in optimizing compilers for imperative languages. Pull arrays make it particularly simple to achieve fusion. It simply amounts to inlining the definitions of functions.

As an example of fusion consider the example `map (*2) (map (*5) arr)`, where each element of the array `arr` is first multiplied by five and then again by two. Conceptually, there is an intermediate array created after the first `map` but thanks to fusion it will be removed. Fusion will proceed as follows:

```

map (*2) (map (*5) arr)
=> { arr }
map (*2) (map (*5) (Pull ixf l))
=> { map }
map (*2) (Pull ((*5) . ixf) l)
=> { map }
Pull ((*2) . (*5) . ixf) l

```

The result is a single Pull array, the intermediate array has been removed.

The correctness of fusion relies crucially on the language being *pure*. If side effects were allowed in the indexing function fusion would not be correct.

There are two different ways of implementing Pull arrays in the literature. The simplest one comes from using Pull arrays in an embedded language, i.e. when the array language is implemented as a library in another host language. Examples of such languages are Pan[11], Feldspar[5], Obsidian[43] and Nikola[24]. By using the technique of implementing Pull arrays as *shallow embeddings* on top of a *deeply embedded* code language, fusion comes completely for free [42].

In the array library Repa[21], compiler supported rewrite rules are used to implement fusion [19].

#### 3.2 Higher dimensions

The first uses of Pull arrays used a fixed number of dimensions, typically either one or two. However, the Repa library introduced a new expressive notion of higher dimensionality for Push arrays [21]. The number dimensions of an array, referred to as the *shape*, are determined statically in the type system. The advantage of having the shape as part of the type is that any program which produces arrays with ill-defined shapes can be ruled out. A potential downside is that enforcing shapes in the type system might be overly constraining and exclude useful programs. A key innovation in Repa is the notion on *shape polymorphism* which makes it possible to write functions which accepts arrays of any shape. Below shows the definition of the type of shapes. It is a variation on how it is represented in Feldspar.

```

data Z
data i :: sh

data Shape sh where
  Z :: Shape Z
  (:.) :: Shape tail -> Int -> Shape (tail :: Int)

```

The first two data declarations introduces new types, `Z` and `::`, without any constructors. They are used to create snoc-lists on the type level, the definition of `Shape`. The type `Shape` is a recursive data type with two constructors. The first constructor `Z` indicates that the shape has zero dimensions. The second constructor `::` adds one dimension to another shape, and stores how many elements there are in that dimension. The type `Shape` has a type parameter which is a snoc list with one element for each dimension.

```

data Pull sh a = Pull (Shape sh -> a) (Shape sh)

```

```

map :: (a -> b) -> Pull sh a -> Pull sh a

```

```
map f (Pull ixf sh) = Pull (f . ixf) sh

zipWith :: (a -> b -> b) ->
          Pull sh a -> Pull sh b -> Pull sh c
zipWith f (Pull ixf1 sh1) (Pull ixf2 sh2)
  = Pull (\sh -> f (ixf1 sh) (ixf2 sh2))
```

## 4. Comparison

### 4.1 Types

### 4.2 $\psi$ -reductions and fusion

### 4.3 Higher dimensions

### 4.4 Functions

MoA	Feldspar
$\delta$	dim . extent
$\varrho$	extent
$\iota \xi^n$	– generalized enumFromTo
$\psi$	index
rav	– flattens to a one-dimensional array
$\gamma$	toIndex
$\gamma'$	fromIndex
$s \hat{\varrho} \xi$	reshape
$\pi x$	product
$\tau$	size
++	++
$\xi_1 f \xi_2$	zipWith f $\xi_1 \xi_2$
$\sigma f \xi$	map f $\xi$
$\xi f \sigma$	map f $\xi$
$\Delta$	take
$\nabla$	drop
$op^{red}$	fold
$\Phi$	reverse
$\Theta$	rotate
$\odot$	– generalized transpose
$f \Omega_d \xi$	– Apply $f$ along the dimension $d$ of $\xi$

### 4.5 Example programs

## 5. Related work

## 6. Future work

## 7. Conclusion

## Acknowledgments

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