A Transformational Approach to Scientific Software: The Mathematics of Array (MoA) Fast Fourier Transform (FFT) with OpenACC

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Abstract

We extend a methodology for designing efficient parallel and distributed scientific software for GPUs introduced in Rosenkrantz et al. [1]. This methodology utilizes sequences of mechanizable algebra-based optimizing transformations. Starting from a high-level algebraic algorithm description in “A Mathematics of Arrays” (MoA) [2], abstract multiprocessor plans are developed and refined to specify which computations are to be done by each processor. Starting with the OpenMP program in Fortran 90 produced in Rosenkrantz et al. [1], we extend it to include OpenACC for GPU support. Our studies show what is needed in OpenACC, support in Fortran compilers for GPUs, and what issues we encountered and resolved.


What is Mathematics of Arrays (MoA)?

- **Mathematics of Arrays (MoA)** is a **theory** of **arrays**, where everything can be written in terms of **array shapes** and **index composition** ("**Psi**" reduction).
- MoA makes an **ideal** formulation of computation when combined with **Lambda calculus** [3].
- Both MoA and Lambda calculus possess the **Church–Rosser property** [4].

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https://surface.syr.edu/eecs_techreports/93/

What is Mathematics of Arrays (MoA)? (cont’d)

- MoA syntax is heavily inspired by the array algebra in 
  Ken Iverson’s APL programming language [5].
- When designing and implementing the APL machine, Phil Abrams introduced the idea of using array shapes [6].
- Lenore Mullin added closure on the algebra [2].


The Cooley–Tukey Fast Fourier Transform (FFT) Algorithm

From van Loan [7], p. 46, Algorithm (1.6.2):

\[
x \leftarrow P_n x
\]

for \( q = 1 : t \)

\[
L \leftarrow 2^t; r \leftarrow n/L
\]

\[
x_{L \times r} \leftarrow B_L x_{L \times r}
\]

end

\[
B_L = \begin{bmatrix} I_{L_0} & \Omega_{L_0} \\ I_{L_0} & -\Omega_{L_0} \end{bmatrix}
\]

\[
\Omega_{L_0} = \begin{bmatrix} 1 \\ \omega_L \\ \vdots \\ \omega_{L_0-1} \end{bmatrix}
\]

In principle, any FFT algorithm could be chosen, but we started with this particular one because:

- It uses **arrays** effectively.
- It uses the **Kronecker product** (= outer product in MoA).
- It is a **simple** operation (1-dimensional radix-2 FFT) that can be easily extended to $N$ dimensions.
- It is one of the **most popular** algorithms for the FFT.
- Van Loan is a respected expert on arrays.
MoA and Transformations

- MoA uses a **systematic, algebraic** design methodology to reduce the FFT algorithm into a semantic **denotational normal form (DNF)**.
- Next, we employ "**dimension lifting**" to get the **operational normal form (ONF)**.
  - It describes the problem and **partitioning** of **data** over **processors** and **memory hierarchies**.
  - It allows one to mathematically prove the **efficiency** and **correctness** of a given algorithm as measured in terms of a set of metrics (such as processor/network/memory speeds).
- Such an approach allows the average programmer to achieve **high-level optimizations** similar to those used by compiler writers, e.g. the notion of tiling.
- We envision scientific programs in the future will be developed in an **interactive** development environment that combines **human judgment** with **compiler-like analysis**, such that transformation and verification of its correctness can be done **mechanically**.
The bit reversal permutation

- Notice the first step of the Cooley-Tukey algorithm is the **bit reversal** permutation $x \leftarrow P_n x$.

- van Loan [7], p. 39, Algorithm (1.5.1):
  
  For $t \geq 1$ and $0 \leq k < 2^t$,
  
  $j \leftarrow 0; m \leftarrow k$
  
  for $q = 0 : t - 1$
  
  $s \leftarrow \text{floor}(m/2)$
  
  $\{b_q = m - 2s\}$
  
  $j \leftarrow 2j + (m - 2s)$
  
  $m \leftarrow s$
  
  end

- We developed this algorithm with MoA:

  $P_n = \mathcal{F} \left( (\langle t \rangle \rho 2) \rho (\nu 2^t) \right)$

- The implementation uses bit shifts:

  ```
  revivec = 0; k = i
  DO j = 1, t
    revivec = ISHFT( revivec, 1 )
    revivec = IOR( revivec, IAND( k, 1_d1 ) )
    k = ISHFT( k, -1 )
  END DO
  revivec = k
  ```

The base CPU-only version

- Rosenkrantz et al. preprint [1] details the rationale and development from the original Cooley-Tukey algorithm to the MoA version.
- The Operational Normal Form (ONF) from MoA enables one to choose the block size that gives the best performance for any individual machine -- assuming intentional information can be processed by a compiler.
- The generic design of the program is then implemented in Fortran with three versions: sequential, shared memory (OpenMP), and distributed memory (MPI).

The GPU-enabled version with OpenACC

- The GPU has its *unique* memory hierarchy, which is arguably a *mix* between shared memory and distributed memory.
  - Device memory is distinct from host memory (unless when using unified memory, which we chose *not* to use).
  - Global device memory is shared between execution units (SMs on NVIDIA, CUs on AMD, etc.)
  - On NVIDIA GPU, CUDA shared memory is shared between threads in the same block.

- For this reason, we start with the *shared memory model* and the OpenMP version of the code, and port it for GPUs using OpenACC.
Why use OpenACC?

- **Ease of use**: just “sprinkle” some directives at the right places, and the code is GPU-enabled!
- Ability to maintain a **single source code** for both the CPU-only and the GPU-enabled versions.
- **Portability**: same code can run on both NVIDIA GPU (pgf90/nvfortran) and AMD GPU (gfortran ≥ 10).

*Rumor has it that Intel GPU support is coming soon too.*
Favorite OpenACC features

- **Full Fortran support** (unlike HIP or DPC++)
- Manual control over grid and block size via num_gangs, num_workers, and vector_length clauses

```
!$acc parallel num_gangs(ngang) num_workers(nworker) vector_length(veclen)
```

116, Generating Tesla code

121, !$acc loop gang(1024) ! blockIdx%x
123, !$acc loop worker(8) ! threadIdx%y
125, !$acc loop vector(128) ! threadIdx%x
Favorite OpenACC features (cont’d)

- Competitive **performance** w.r.t. CUDA on NVIDIA GPUs

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</table>
Favorite OpenACC features (cont’d)

- cache directive for using CUDA shared memory

```c
!$acc loop vector collapse(2) private( c, d ) independent
do i = 0, size-1, Lnew
  do j = 0, (Lnew/2)-1
    !$acc cache( weight_p, zblock_p )
    c = weight_p(j) * zblock_p( i + j + Lnew/2 )
    d = zblock_p( i + j )
    zblock_p( i + j ) = d + c
    zblock_p( i + j + Lnew/2 ) = d - c
  end do ! j
end do ! i
```
OpenACC wishlist

- **Array reduction** over an arbitrary axis (supposedly introduced in OpenACC 2.7, but we can’t seem to get it to work...)

```fortran
integer :: i, j, m, n
real, allocatable :: vec(:,), mat(:, :)
allocate( vec(m), mat(m, n) )
!$acc data create( vec, mat )

!$acc parallel
!$acc loop gang
do i = 1, m
  vec(i) = 0.0
  !$acc loop vector reduction(+:vec)
  do j = 1, n
    vec(i) = vec(i) + mat(i, j)
  end do
end do
```
OpenACC wishlist

- **Array reduction** over an arbitrary axis  
  (supposedly introduced in OpenACC 2.7, but we can’t seem to get it to work…)

- Manual **synchronization** routines

  ```
  __syncwarp()
  __syncthreads()
  cudaStreamSynchronize() == !$acc wait
  cudaDeviceSynchronize()
  ```
OpenACC wishlist

- **Array reduction** over an arbitrary axis (supposedly introduced in OpenACC 2.7, but we can’t seem to get it to work…)
- Manual **synchronization** routines
- No “**hidden**” cost of OpenACC runtime library initialization

```fortran
! Notice we have moved OpenACC runtime ! initialization (~300 ms) outside of ! the timing region for initialization

(!$acc init

t0 = now()
do i = 0, n - 1
   z(i)= cmplx( i, 0._dd, kind=dz )
end do

t1 = now()
time_init = t1 - t0
```
OpenACC wishlist

- **Array reduction** over an arbitrary axis
  (supposedly introduced in OpenACC 2.7, but we can’t seem to get it to work...)
- Manual **synchronization** routines
- No “**hidden**” cost of OpenACC runtime library initialization
- Support for **pinned memory**

```fortran
! CUDA Fortran
ATTRIBUTES(pinned) :: x
```
OpenMP target offload?

- Once compiler support matures for OpenMP target offload, we will consider porting from OpenACC into OpenMP target offload.
- Doing this would enable **concurrent parallelism** for both multicore CPUs and accelerators (GPUs) under the **same programming model**.
- Automated **runtime translation** tools (e.g. clacc and flacc [8]) are welcome too!

[8] [https://csmd.ornl.gov/project/clacc](https://csmd.ornl.gov/project/clacc)
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