Los Alamos
NATIONAL LABORATORY

General purpose GPU programming made easy

Nathaniel Morgan[1], Erin Heilman [1], Calvin Roth [1], and Caleb Yenusah[1]

Contributors: Robert Robey[2], Daniel Dunning[1,2], Adrian Diaz[1], Jacob Moore[1], Tanya Tafolla[1], Eappen Nelluvelil[1], and Russel Marki [1]

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[1]X-Computational Physics: Continuum Models and Numerical Methods

[2]X-Computational Physics: Eulerian Codes

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Introduction

GPUs are designed to perform mathematical operations in parallel

- CPUs are designed for intricate work flows and diverse applications
- GPUs have significantly more arithmetic logic units (ALU) or float point units (FPUs) than CPUs, compare the green boxes in the Figure
- CPUs have more cache memory than GPUs

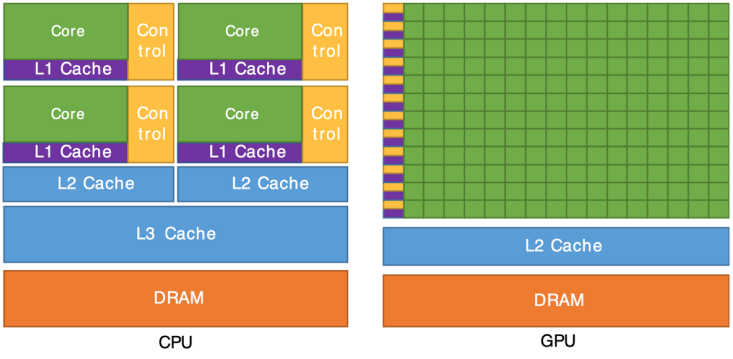
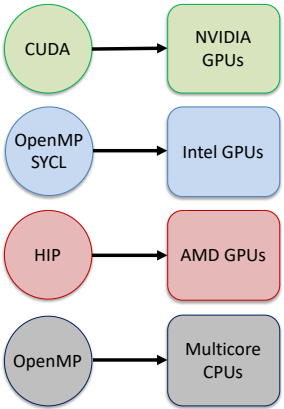


Figure: Comparison of GPU and CPU architectures[1]

[1] Image is from `https://cvw.cac.cornell.edu/GPUarch/gpu_characteristics`

CPUs and GPUs have vendor specific fine-grained parallelism languages



Plus openCL and openACC

The Kokkos [2] performance portability library:

- Enables a single implementation to run on all architectures - replaces vendor specific languages
- Is based solely on C++11 (no special compiler language needed!)
- Has capabilities to manage access, allocation, and copying of data between CPU and GPU

Goals for this work:

- Enable easy adoption of data oriented programming (DOP) in codes
- Simplify the use of Kokkos in a code (C++ or Fortran) and extend it to support sparse data representations

The C++ MATrix and ARray (MATAR) library is written using Kokkos for performance, portability, and productivity

- MATAR [1] is designed to support dense and sparse data representations using DOP following the C++17 standard.
- MATAR addresses:
  - Performance: contiguous dense and sparse data representation (i.e., use DOP).
  - Portable: run across CPUs and GPUs (using `Kokkos`) with a single implementation.
  - Productivity: easy to create, use, and integrate into codes (C++ and Fortran). For data allocating types,the memory is managed for the user.
- MATAR works in partnership with MPI or data management frameworks (e.g., FleCSI)

MATAR design philosophy

- Enable a coding syntax that looks similar to C, python, and Fortran while adhering to C++
- Eliminate all parallel language syntax in a code (no pragmas, no Cuda, etc.)
- Enable existing codes to run on CPUs and GPUs after minor changes to the syntax

MATAR data types

MATAR has a rich set of capabilities to support diverse computational physics applications

Dense data representations include:

		Indexing pattern	
		0-indexed	1-indexed
Access pattern	Column major	FArrayKokkos ViewFArrayKokkos DFArrayKokkos DViewFArrayKokkos	FMatrixKokkos ViewFMatrixKokkos DFMatrixKokkos DViewFMatrixKokkos
	Row major	CArrayKokkos ViewCArrayKokkos DCArrayKokkos DViewCArrayKokkos	CMatrixKokkos ViewCMatrixKokkos DCMatrixKokkos DViewCMatrixKokkos

Sparse data representations include:

		Indexing pattern
		0-indexed
Access pattern	Column major	RaggedDownArrayKokkos DynamicRaggedDownArrayKokkos CSCArrayKokkos
	Row major	RaggedRightArrayKokkos DynamicRaggedRightArrayKokkos CSRArrayKokkos

There are more data types than shown in these tables

MATAR offers many allocatable data types on GPUs

MATAR 3D array example

```
// allocate 10x10x10 array on the GPU
CArrayKokkos <int> array3D (10,10,10);
```

```
// use array3D on the GPU
array3D(i,j,k) = 1;
```

MATAR 2D dual-array example

```
// allocate a 4x5 array on the CPU and GPU
DCArrayKokkos <double> array2D (4,5);
```

```
// use array2D on the CPU (host)
array2D.host(i,j) = 3.45;
```

```
// use array2D on the GPU (device)
array2D(i,j) = 3.45;
```

```
// methods to copy data
array2D.update_device(); // update GPU
array2D.update_host(); // update CPU
```

MATAR offers many data types to view data as multidimensional on GPUs

MATAR view of a 2D array example

```
// ...
// coding run on the GPU
// ...

int A[9];
ViewCArrayKokkos <int> array2D (&A[0],3,3);

// use array2D
array2D(i,j) = 1;
```

MATAR offers many types to view data as multidimensional on multi-core CPUs and GPUs

MATAR dual view of a 2D array example

```
// on the CPU
int A[27]; // can be an array from an existing MPI code etc.
DViewCArrayKokkos <int> array3D (&A[0],3,3,3);

// use array3D on the CPU (host)
array3D.host(i,j,k) = 3;
```

```
// use array3D on the GPU (device)
array3D(i,j,k) = 4;
```

```
// methods exist to update GPU or CPU array3D
array3D.update_host();
```

Simple syntax to slice or create a data access pattern with existing allocated arrays or matrices

```
// allocate num_cellsx3x3 stress
int num_cells = 100000;
CArrayKokkos <double> cell_stress (num_cells,3,3);
```

MATAR slice of an array

```
// inside a routine run on a GPU
// slice out the stress in a cell
int cell_id=314;  // cell id
ViewCArrayKokkos <double> stress (&cell_stress(cell_id,0,0),3,3);

// Use stress
for (int i = 0; i < 3; i++) {
    stress(i,i) = -pressure;
} // end for loop
```

MATAR parallel loops

MATAR provides simple to use syntax to run loops in parallel on both multi-core CPUs and GPUs

C++ MATAR 3D array example

```
// allocate 10x10x10 array
CArrayKokkos <int> array3D (10,10,10);

// DOP parallel loop using MATAR+Kokkos
FOR_ALL (i, 0, 10,
         j, 0, 10,
         k, 0, 10, {
            array3D(i,j,k) = 1;
}) // end parallel for loop

// runs in parallel on GPUs and CPUs
// leveraging Kokkos
```

Classic 3D C++ array example

```
// allocate 10x10x10 array
int array3D [10][10][10];

// Classic 3D for loop
for (int i = 1; i < 10; i++) {
    for (int j = 1; j < 10; j++) {
         for (int k = 1; k < 10; k++){
            array3D[i][j][k] = 1;
        }
    }
} // end for loop
```

Simple syntax is key to having maintainable coding

C++ MATAR 2D array example

```
// allocate 10x10 array
CArrayKokkos <int> array2D(10,10);

// Initialize matrix3D in parallel
FOR_ALL (i, 0, 10,
         j, 0, 10, {
            array2D(i,j) = 1;
}); // end parallel for
// array2D is on the e.g., GPU
```

The Kokkos syntax is powerful but not straightforward to use. MATAR greatly simplifies using Kokkos in a code.

Kokkos 2D array example

```
using LoopOrder = Kokkos::Iterate::Right;
using Layout = Kokkos::LayoutRight;
using ExecSpace = Kokkos::Cuda;
using MemoryTraits = void;
// allocate 10x10 array
Kokkos::View<int**, Layout, ExecSpace,
             MemoryTraits> Array2D(10,10);
// Initialize matrix3D
Kokkos::parallel_for(
        Kokkos::MDRangePolicy
        <Kokkos::Rank<2,LoopOrder,LoopOrder>>
        ( {0, 0}, {10, 10} ), KOKKOS_LAMBDA
        ( const int i, const int j ){
            array2D(i,j) = 1;
        });
// array2D is on the e.g., GPU
```

MATAR supports a myriad of parallel loop types on a GPU

C++ parallel loop examples

```
// all loops go from i=a to i<N
FOR_ALL();
REDUCE_SUM();
REDUCE_MAX();
REDUCE_MIN();
```

Fortran-like parallel loop examples

```
// all loops go from i=a to i<=N
DO_ALL();
DO_REDUCE_SUM();
DO_REDUCE_MAX();
DO_REDUCE_MIN();
```

Serial execution

```
// run coding serially on a GPU
RUN();
```

Using MATAR with Fortran codes

MATAR supports Fortran multidimensional dense data access patterns and indexing

	j = 0	j = 1	j = 2	j = 3
i = 0	10.9	0.9	11.3	90
i = 1	0.5	110.1	0.125	81
i = 2	1.2	7.3	8.19	14.12
i = 3	8.9	45.1	1	11.9

Index	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
Data	10.9	0.5	1.2	8.9	0.9	110.1	7.3	45.1	11.3	0.125	8.19	1	90	81	14.12	11.9

Figure: The data inside MATAR is 1D but accessed as $A(i, j)$ contiguously.

The goal with MATAR is to make GPU coding as simple as possible

C++ MATAR 3D matrix example

```
// allocate 10x10x10 matrix
FMatrixKokkos <int> matrix3D (10,10,10);

// Initialize matrix3D in parallel
DO_ALL (k, 1, 10,
        j, 1, 10,
        i, 1, 10, {
            matrix3D(i,j,k) = 1;
}); // end parallel do
// matrix3D is on the device, e.g., GPU
```

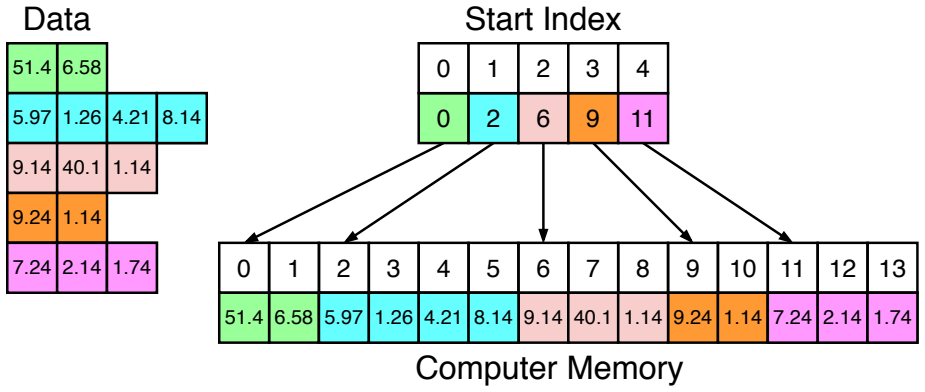
Fortran 3D matrix example

```
! allocate 10x10x10 matrix
INTEGER :: matrix3D (10,10,10)

! Initialize matrix3D
DO k = 1, 10
    DO j = 1, 10
        DO i = 1, 10
            matrix3D(i,j,k) = 1
        END DO
    END DO
END DO
```

MATAR sparse types

MATAR supports a ragged-right sparsity type



The layout of a ragged-right array where the column size for each row varies. The user accesses the data as a 2D array, $A(i, j)$, but the data in memory is stored as a contiguous 1D array by rows.

Simple-to-use sparse data representations benefit computational physics codes

Consider the ragged-right array,

$$\mathbf{R}(i,j) = \begin{matrix} (1 & 1 & 1) \\ (2 & 2) \\ (3) \\ (4 & 4 & 4 & 4) \end{matrix}$$

C++ MATAR ragged-right example

```
CArrayKokkos <int> set_strides(4);
RUN({set_strides(0)=3;
     set_strides(1)=2;
     set_strides(2)=1;
     set_strides(3)=4;
    }); // serial execution on a GPU

RaggedRightArrayKokkos <int> my_ragged(set_strides);

FOR_ALL (i, 0, 4, {
    for (int j = 0; j < my_ragged.stride(i); j++){
        my_ragged(i,j) = i;
    }
}); // end parallel for loop
```

MATAR extends Kokkos to support performance portability with diverse sparse data types

C++ MATAR example using Kokkos

```
int i_max = 3, j_max = 5;

DynamicRaggedRightArrayKokkos <int> my_dyn_ragged(i_max, j_max);

// parallel for loop on a CPU or GPU using MATAR+Kokkos
FOR_ALL(i, 0, i_max, {
    for (int j = 0; j <= (i % j_max); j++) {
        my_dyn_ragged.stride(i)++;
        my_dyn_ragged(i,j) = j;
    } // end for
}); // end parallel for
Kokkos::fence();  // wait for all threads to finish
```

MATAR supports a large suite of data representations, only a few are presented in this talk

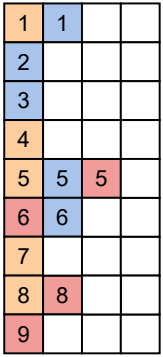
Dense data types include

FArrayKokkos	ViewFArrayKokkos
FMatrixKokkos	ViewFMatrixKokkos
CArrayKokkos	ViewCArrayKokkos
CMatrixKokkos	ViewCMatrixKokkos
DFArrayKokkos	DViewFArrayKokkos
DFMatrixKokkos	DViewFMatrixKokkos
DCArrayKokkos	DViewCArrayKokkos
DCMatrixKokkos	DViewCMatrixKokkos

Sparse data types include

RaggedRightArrayKokkos	RaggedRightArrayVectorsKokkos
RaggedDownArrayKokkos	CSRArrayKokkos
DynamicRaggedRightArrayKokkos	CSCArrayKokkos
DynamicRaggedDownArrayKokkos	

There are more data types than shown in these tables



The dynamic ragged arrays have memory buffers. The dynamic ragged-right is shown.

MATAR supports sparse arrays with similar support as the scipy sparse CSR and CSC matrix types

C++ MATAR coding

```
int column_arr[] = {0, 2, 2, 0, 1, 2};
CArrayKokkos <double> data(6);
CArrayKokkos <int> row(4);
CArrayKokkos <int> column(6);
RUN ({
    for(int i = 0; i < 6; i++){
        data(i) = i+1.5;
        column(i) = column_arr[i];
    } // end for
    row(0) = 0;
    row(1) = 2;
    row(2) = 3;
    row(3) = 6;
});
CSRArrayKokkos <double> A(data, row, column,
                          3, 3);
```

python coding

```
column_arr =  [0, 2, 2, 0, 1, 2];
data = np.zeros((6,), dtype=np.float64);
row = np.zeros((4,), dtype=np.uint32);
column = np.zeros((6,), dtype=np.uint32);

for  i in range(6):
    data[i] = i+1.5;
    column[i] = column_arr[i];
row[0] = 0
row[1] = 2
row[2] = 3
row[3] = 6

A = csr_matrix((data, column, row),
                shape=(3,3), dtype=np.float64)
```

General examples

Example: passing MATAR data types to functions

coding

```
int calculate_sum(const FMatrixKokkos<int> &matrix){
   int local_sum;
   int sum;

   // do summation in parallel on GPU
   DO_REDUCE_SUM(k, 1, 6,
                 j, 1, 5,
                 i, 1, 4,
                 local_sum, {
                     local_sum += matrix(i,j,k);
                 }, sum);
    return sum;
} // end function
```

Example: Enumerated lists on a GPU

header file

```
// enum
namespace choices
{
    enum myChoice
    {
        METHOD_A = 1,
        METHOD_B = 2,
        METHOD_C = 3
    };
}
```

coding

```
CArrayKokkos <choices::myChoice> my_choices(2);

// set the method on the GPU
RUN({
        my_choices(0) = choices::METHOD_A;
        my_choices(1) = choices::METHOD_B;
});

FOR_ALL(i,1,2,{
    switch (my_choices(i)) {
        case choices::METHOD_A: { // do stuff
            break;}
        case choices::METHOD_B: { // do stuff
            break;}
    }; // end switch
});
```

Example: Using MATAR with structs and classes

header file

```
// a struct with dual arrays inside
struct cell_data_t{

    DCArrayKokkos <double> den;
    DCArrayKokkos <double> pres;

    KOKKOS_FUNCTION
    void initialize(const int i,
                    const int j,
                    const int k) const{
        den(i,j,k)  = 0.0;
        pres(i,j,k) = 0.0;
    };
};
```

coding

```
cell_data_t cell_data;

cell_data.den =
    DCArrayKokkos <double> (10,10,10);
cell_data.pres =
    DCArrayKokkos <double> (10,10,10);

// initialize cell variables on GPU
FOR_ALL(i, 0, 10,
        j, 0, 10,
        k, 0, 10, {
        // remember KOKKOS_FUNCTION
        cell_data.initialize(i,j,k);
    });
```

Example: Using function pointers on a GPU for object-based programming

header file

```
// function pointer
template <typename T>
struct method_ptrs{
  void (*fcn_ptr)(const T);
};

template <typename T>
KOKKOS_FUNCTION
void sum(const T){ };

template <typename T>
KOKKOS_FUNCTION
void multiply(const T){ };
```

coding

```
CArrayKokkos <method_ptrs<FMatrixKokkos<int>>>
                                        Array_ptrs(2);
// set the pointer on the device e.g., GPU
RUN({
    Array_ptrs(0).fcn_ptr = sum;
    Array_ptrs(1).fcn_ptr = multiply;
});
Kokkos::fence();

// use the function
FOR_ALL(i,0,2, {
    Array_ptrs(i).fcn_ptr(matrix2D);
});
```

Example: Adding MATAR to an existing MPI code

Struct in existing code

```
// The data in an existing code
struct code_t{
    double data1[100];
    double data2[100];
};
```

header file

```
// MATAR view of the existing data
struct code_matar_t{
   DViewCArrayKokkos <double> data1;
   DViewCArrayKokkos <double> data2;
};
```

coding

```
code_matar_t mtr;

mtr.data1 = DViewCArrayKokkos
      <double> (&code.data1[0],10,10);
mtr.data2 = DViewCArrayKokkos
      <double> (&code.data2[0],10,10);

// set the code values on the GPU
FOR_ALL(i, 0, 10,
        j, 0, 10, {
            mtr.data1(i,j) = 5.6;
            mtr.data2(i,j) = 9.2;
        });
Kokkos::fence();
mtr.data1.update_device(); // code_t data1
mtr.data2.update_device(); // code_t data2
```

Additional examples

Example: Half-space cooling model for oceanic lithosphere

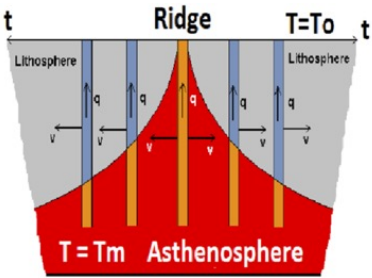


Figure: Illustration of simulation

$$T(t,z) = T_m \mathrm{erf}(z(4\kappa t)^{-1/2})$$

```
DynamicRaggedDownArrayKokkos <double>
                    dyn_ragged_down(max_age+1, depth+1);
DO_ALL(i, 0, max_age, {
    for (int j = 0; j <= depth; j++) {
        if (i == 0 && j == 0){
            dyn_ragged_down.stride(j)++;
            dyn_ragged_down(i, j) = mantle_temp;
        } // end if
        double temp = mantle_temp *
                erf(j/(2.0*sqrt(thermal_diff*(i*1e6))));
        dyn_ragged_down.stride(j)++;
        dyn_ragged_down(i, j) = temp;

        // check if we have reached the mantle
        if (round(dyn_ragged_down(i, j)) == 1350) break;
    } // end for
}); // end parallel DO_ALL
```

Very favorable GPU run times are achieved for the half-space cooling simulation

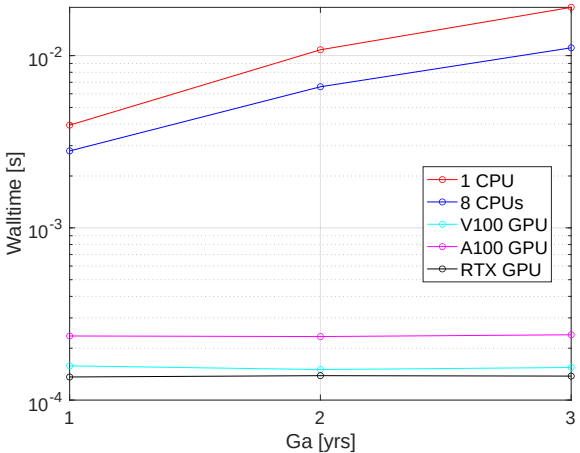


Figure: 1 RTX GPU gives approximately 100X acceleration over serial at t=3 Ga yrs

Watts-Strogatz graph: Find the average shortest distance between nodes

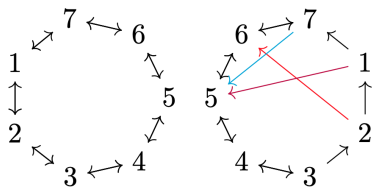


Figure: On the left, ring lattice with 7 elements where each node is connected to it's nearest 1 neighbor. On the right we replace three edges with random edges.

```
for (k = 0; k < n_nodes; k++){
    FOR_ALL(i, 0, n_nodes,
            j, 0, n_nodes, {
            if(i != j){
                int dist1 = res(i,k) + res(k,j);
                int dist2 = res(i,j);
                if(dist1 < 0){
                    dist1 = INT_MAX;
                }
                if(dist2 < 0){
                    dist2 = INT_MAX;
                }
                if(dist1 < dist2){
                    res(i,j) = dist1;
                }
            } // end if
    }); // end parallel for
} // a parallel reduction follows to get an average
```

MATAR enables 2460X acceleration on a GPU over serial python for the Watts-Strogatz graph calculation

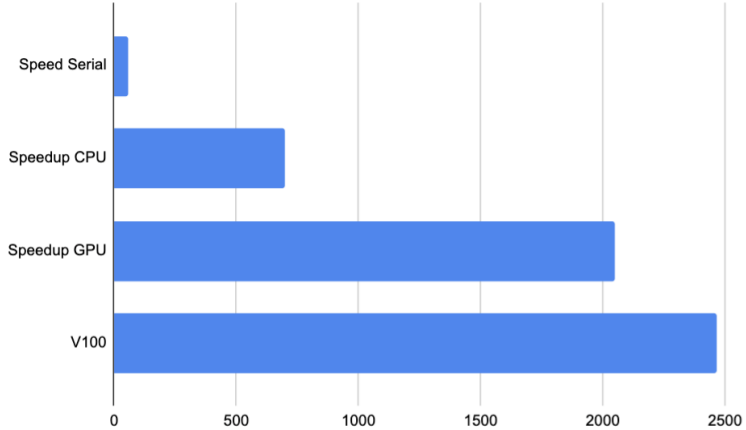


Figure: Compared to python, serial MATAR is 60x faster, 16 threads on a CPU is about 700x faster, a Titan GPU is about 2050x faster, and a V100 GPU is 2460X faster.

Lagrangian hydrodynamics

The Fierro Lagrangian hydrodynamic code contains continuous and discontinuous finite element methods

1D hydro code snippet from the Fierro GitHub repository

```
 // v_new = v_n + alpha*dt/mass*Sum(forces)
FOR_ALL (node_id, 1, num_nodes-1, {

    int corner_id_0 = get_corners_in_node(node_id, 0); // left corner id
    int corner_id_1 = get_corners_in_node(node_id, 1); // right corner id

    double force_tally = corner_force(corner_id_0) +
                         corner_force(corner_id_1);

    // update velocity
    node_vel(node_id) = node_vel_n(node_id) +
                        rk_alpha*dt/node_mass(node_id)*force_tally;

}); // end parallel for on device
```

The Fierro code has 2D-RZ & 3D Lagrangian hydrodynamic methods written with MATAR that run on CPUs and GPUs

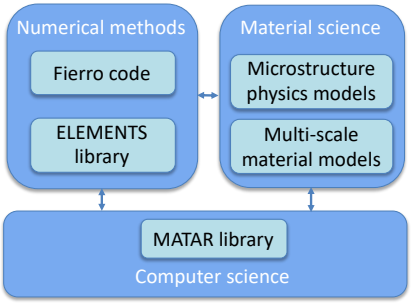
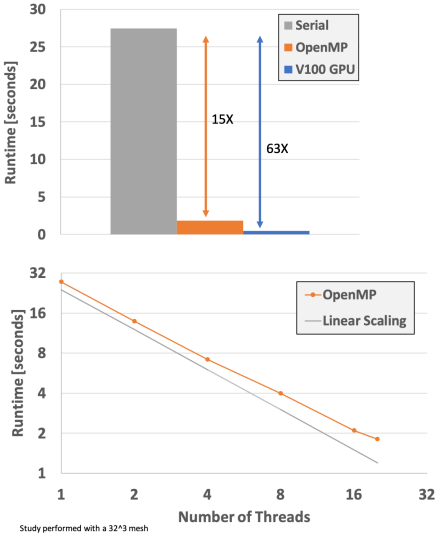


Figure: The code structure



The Fierro code has diverse finite element methods covering quasi-static to shock-driven material dynamics

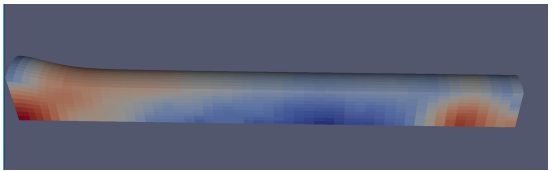


Figure: A parallel Taylor Anvil simulation using a hypo-elastic plastic model and an analytic equation of state with Fierro on a 6307 element mesh

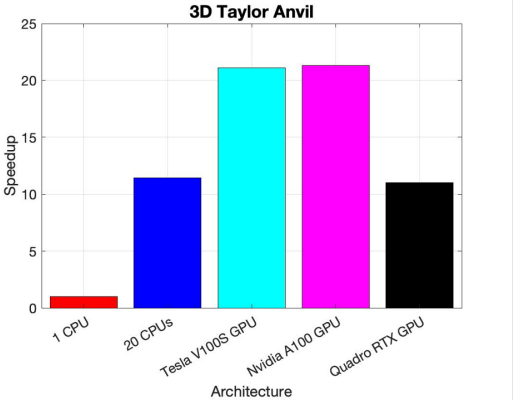


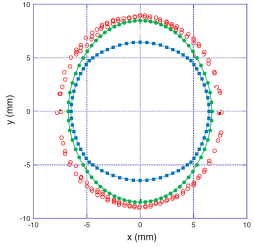
Figure: GPUs can deliver reasonable speed-ups, even with a coarse mesh resolution, on the Taylor Anvil simulation, see image on the left

The visco-plastic self-consistent generalized material model (VPSC-GMM) was quickly updated using MATAR

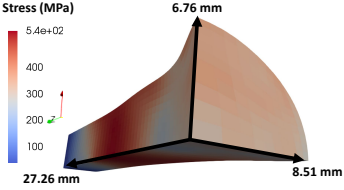
- VPSC-GMM is a scale-bridging material model with ∼20K lines of Fortran code.
- Converted to C++ using MATAR in 2 weeks
- VPSC-GMM is running on CPUs and GPUs

Taylor Anvil Simulation Results at 100 µs

Calculated cross section of the rod using the PTW model (blue) and the VPSC model (green) compared with the data (red)



Calculated von Mises stress at 100 µs using the VPSC model



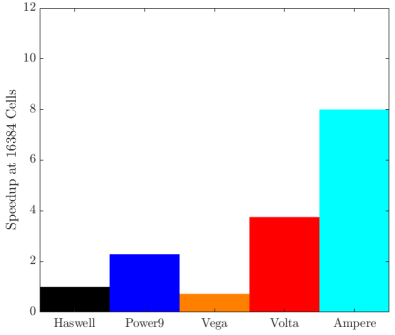
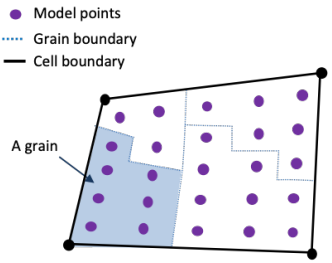


Figure: MATAR+Kokkos delivers performance portability over CPUs and GPUs

GPUs enable more timely simulations with high-fidelity multi-scale material models



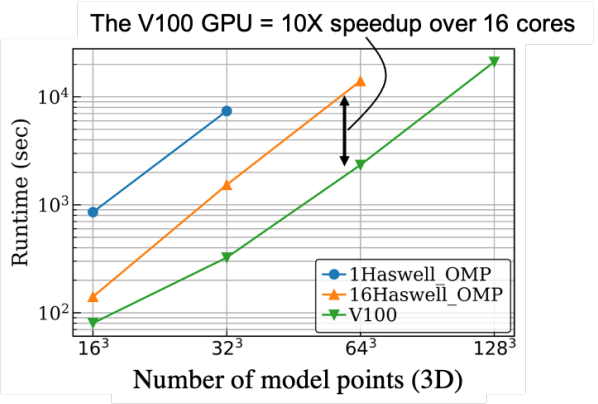


Figure: The 3D elasto-viscoplastic (EVP-FFT) multi-scale model was rewritten using MATAR to run across CPU and GPU architectures

Conclusions

MATAR is designed to help people write codes that run in parallel across CPUs and GPUs

- MATAR uses DOP for **P**erformance, Kokkos for **P**ortability over architectures, and uses simple interfaces for **P**roductivity —3P's in writing software.
  - Contains many data types including dense and sparse types
  - Can benefit existing or new C++ codes, and aids conversion of existing Fortran routines to C++ with Kokkos
  - Successfully used in diverse applications including contact surface detection, phase-field modeling, scale-bridging material models, finite element solvers, discontinuous Galerkin methods, and more.
- MATAR (for parallelism on CPUs or GPUs): https://github.com/lanl/MATAR
- ELEMENTS (finite element library): https://github.com/lanl/ELEMENTS
- Fierro (Implicit and explicit FE code): https://github.com/lanl/Fierro

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Domain-Specific Languages and High-Level Frameworks for High-Performance Computing.