# Accelerating Biomedical Data Science with GPUs: Practical Approaches and Tools

## Minerva Scientific Computing Environment

https://labs.icahn.mssm.edu/minervalab

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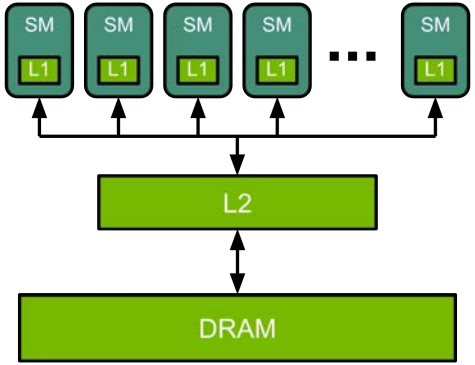
Sinai

# Outline

- GPU Architecture Fundamentals
- Ways to Accelerate with GPUs
  - Application-Based Solutions
  - GPU-Optimized Libraries
  - OpenACC Directives
  - CUDA Programming
  - Standard Language Parallelism

# Graphics Processing Unit (GPU) Architecture Fundamentals

- GPUs are equipped with thousands of smaller, efficient cores that can perform simple tasks in parallel
- Key Architectural Components:
  - **Streaming Multiprocessors (SMs)**
    - The core computational units of a GPU
    - Each SM contains multiple CUDA cores, responsible for parallel data processing
    - SMs have their own L1 cache to store frequently accessed data and shared memory for fast data sharing between threads
    - Warp scheduling: SMs execute instructions in parallel, typically in groups of 32 threads (warps), which helps maximize throughput
  - **L2 Cache**
    - Shared by all SMs, which improves data access efficiency when multiple SMs need the same data
  - **High-Bandwidth DRAM**
    - Used for storing data
    - Data is fetched from DRAM to SMs via the L2 and L1 caches to optimize memory bandwidth usage




https://docs.nvidia.com/deeplearning/performance/dl-performance-gpu-background/index.html

# GPU Architecture Fundamentals

- Multiply-Add Operations:
  - One of the most frequent operations in neural networks is **multiply-add**, used to compute dot products in fully-connected and convolutional layers
  - GPUs are optimized for these operations, with each multiply-add operation counting as two floating-point operations (FLOPs). Modern GPUs can process millions to billions of these operations per second, making them ideal for AI and machine learning applications that require high computational throughput
- Tensor Cores and CUDA Cores:
  - **Tensor Cores** (introduced in Volta architecture) are specialized units for accelerating matrix multiplications, critical for machine learning
  - **CUDA Cores** handle general-purpose computing tasks when operations do not fit the matrix multiplication model, such as element-wise operations

# Ways to Accelerate with GPUs

- Application-Based Solutions
  - Directly leverage pre-built applications for immediate results
- GPU-Optimized Libraries
  - Utilize high-performance libraries for seamless acceleration
- OpenACC Directives
  - Simplify code modifications to accelerate existing applications easily
- CUDA Programming
  - Gain maximum performance through custom GPU code development
- Standard Language Parallelism
  - Flexibly integrate GPU acceleration using standard parallelism techniques

# Ways to Accelerate with GPUs: Application-Based Solutions

# Key Applications Across Industries

| Industry | Popular GPU-Accelerated Applications |
|---|---|
| **Artificial Intelligence** | PyTorch, MXNet, TensorFlow, Caffe, Keras, Scikit-learn, ONNX, DeepStream |
| **Climate & Weather** | Cosmos, Gales, WRF, MPAS, NEMS, RegCM, GEM, ICON |
| **Computational Finance** | O-Quant Options Pricing, Murex, MISYS, Numerix, GPUdb, RiskVal, CuQuant |
| **Data Science & Analytics** | Anaconda, H2O, OmniSci, RAPIDS, Dask, XGBoost, TensorRT, cuML |
| **Federal Defense & Security** | ArcGIS Pro, EVNI, SocetGXP, Cylance, FaceControl, Raytheon, Harris Geospatial, TensorVision |
| **Life Sciences** | Amber, LAMMPS, GROMACS, NAMD, Relion, VASP, AlphaFold, SCHRODINGER |
| **Manufacturing & Engineering** | Ansys Fluent, Abaqus SIMULIA, AutoCAD, CST Studio Suite, Altair, Simcenter, OpenFOAM, NASTRAN |
| **Media & Entertainment** | DaVinci Resolve, Premiere Pro CC, Redshift Renderer, Autodesk Maya, Blender, Nuke, Unreal Engine, 3ds Max |
| **Medical Imaging** | Aidoc, PowerGrid, RadiAnt, NVIDIA Clara, Arterys, iCAD, Visage, Philips IntelliSpace |
| **Oil & Gas** | Echelon, RTM, SPECfem3D, Paradigm, Schlumberger Eclipse, PetroMod, JewelSuite, GeoTeric |
| **Retail** | Everseen, Deep North, Third Eye Labs, AWM, Malong, Clarifai, Antuit, Google Cloud AI |
| **Supercomputing & HPC** | Chroma, GTC, MILC, QUDA, XGC, HPL, NWChem, VMD, BerkeleyGW |

https://www.nvidia.com/en-us/accelerated-applications/

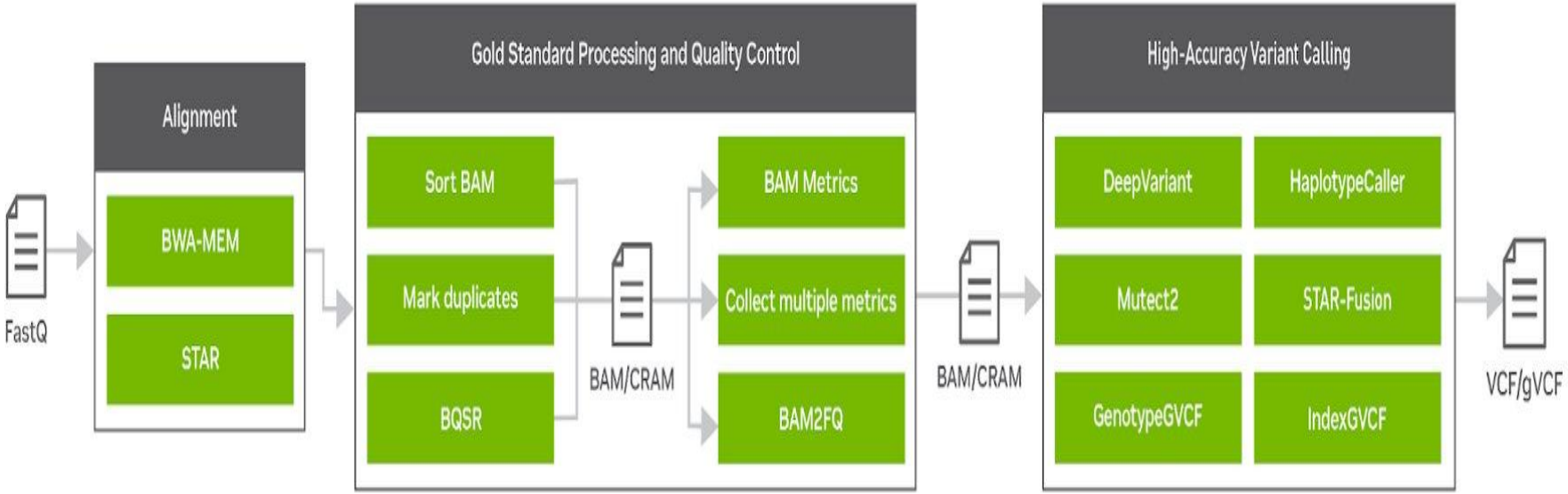
# Performance Gains of Standard Benchmarks: A100 vs Dual CPU

| Application | Speedup on A100 vs Dual CPU |
|---|---|
| Amber | 13x – 39x |
| GROMACS | 6x – 9x |
| LAMMPS | 5x – 18x |
| NAMD | 6x – 8x |
| Relion | 4x – 5x |
| Chroma | 32x |
| GTC | 14x |
| MILC | 32x |
| SPECfem3D | 29x |
| FUN3D | 13x |

https://labs.icahn.mssm.edu/minervalab/wp-content/uploads/sites/342/2024/05/FiveWays-HealthCare-April2024.pdf

https://developer.nvidia.com/hpc-application-performance

# NVIDIA Parabricks for Alignment & Variant Calling




https://developer.nvidia.com/blog/new-research-highlights-speed-and-cost-savings-of-clara-parabricks-for-genomic-analyses/

# NVIDIA Parabricks for Alignment & Variant Calling

- **Alignment (BWA-MEM, Minimap2, STAR)**
  - **GPU:** 11 minutes | **CPU:** ~4 hours
  - Input: FastQ files
- **Gold Standard Processing & Quality Control (Sort BAM, Mark Duplicates, BQSR)**
  - **GPU:** 6 minutes | **CPU:** ~9 hours
  - Metrics: BAM Metrics, Collect Multiple Metrics
  - Input/Output: BAM/CRAM
- **High-Accuracy Variant Calling (DeepVariant, HaplotypeCaller, Mutect2)**
  - **GPU:** 4-45 minutes | **CPU:** ~16-31 hours
  - Output: VCF/gVCF files

https://labs.icahn.mssm.edu/minervalab/wp-content/uploads/sites/342/2024/05/FiveWays-HealthCare-April2024.pdf

# NVIDIA BioNeMo

- NVIDIA BioNeMo is a generative AI platform for drug discovery that simplifies and accelerates the training of models on proprietary data, ensuring easy, scalable model deployment for drug discovery applications
- **Key Features**:
  - **LLM for Proteins & Molecules**: BioNeMo leverages transformer-based LLMs for biological and chemical data, including proteins, DNA, and small molecules
  - **Pretrained Models**: Offers access to pre-trained AI models optimized for tasks such as molecular property prediction, sequence generation, and structure-based drug design
  - **Custom Model Training**: Supports fine-tuning of models on proprietary datasets to meet specific research goals
  - **Integration**: Easily integrates with NVIDIA's GPU-accelerated platforms like Clara and AI frameworks, offering massive parallel processing capabilities

https://www.nvidia.com/en-us/clara/bionemo/

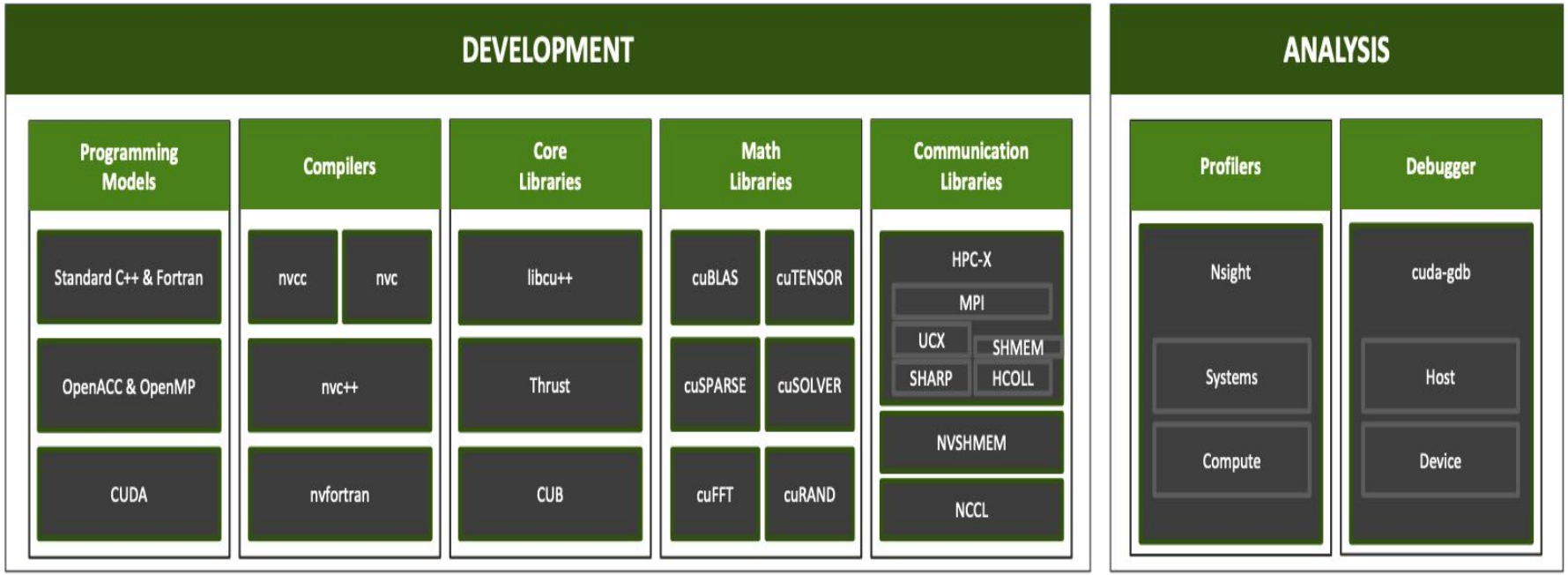
# NVIDIA BioNeMo

- **MegaMolBART:** A model for generating and learning representations of small molecules, useful in drug discovery and chemistry
- **ESM-2nv 3B:** A large protein model that predicts protein properties and aids in structure prediction and functional annotation
- **EquiDock DB5 Model:** Predicts protein-protein interactions, essential for understanding biological processes and drug design
- **DiffDock Score Model:** Generates ligand poses for drug-protein interactions, improving drug discovery efforts
- **Geneformer:** Analyzes single-cell gene expression, advancing research in personalized medicine and developmental biology

https://docs.nvidia.com/bionemo-framework/latest/

# Ways to Accelerate with GPUs: GPU-Optimized Libraries

# NVIDIA HPC Software Development Kit (SDK)

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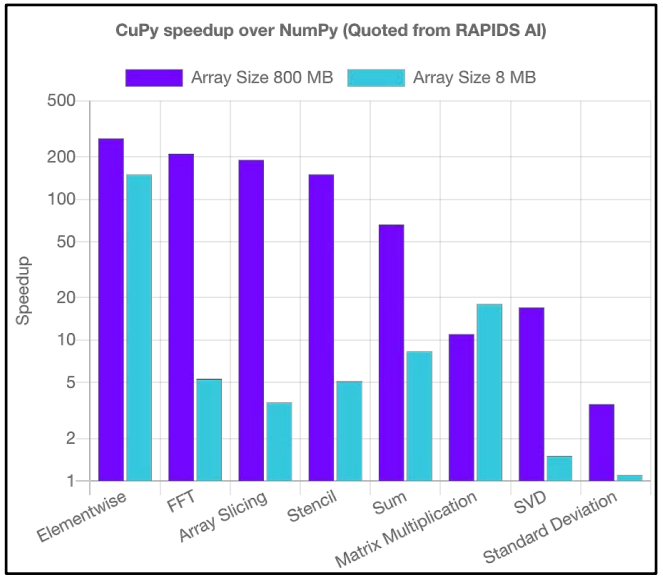
# GPU-Accelerated Libraries

- **Linear Algebra Libraries**
  - *cuBLAS*: Basic Linear Algebra Subroutines
  - *cuBLASLt, cuBLASMp, cuBLASDx*: Lightweight, multi-process, and device-side BLAS extensions
  - *cuTENSOR, cuTENSORMg*: Tensor linear algebra, including multi-GPU support
- **Linear Solvers & Sparse Matrix Operations**
  - *cuSOLVER, cuSOLVERMp*: Dense and sparse direct solvers
  - *cuSPARSE, cuSPARSELt*: Sparse matrix BLAS and lightweight variants
- **Fourier Transform & Random Numbers**
  - *cuFFT, cuFFTMp, cuFFTDx*: Fast Fourier Transform variants
  - *cuRAND*: Random number generation
- **Image, Video, and Compression**
  - *NPP, NPP+*: Image, video, and signal processing
  - *nvJPEG, nvJPEG2000, nvTIFF*: JPEG and TIFF encode/decode
  - *nvCOMP*: Data compression/decompression

https://github.com/nvidia/cudalibrarysamples

# CuPy: GPU-Accelerated Python Library

- **Overview**: Open-source library that accelerates Python computations using NVIDIA CUDA for high performance on GPUs
- **Performance**: Achieves up to 100x speedups in tasks like linear algebra, deep learning, and random number generation
- **NumPy/SciPy Compatible**: Functions as a drop-in replacement for NumPy and SciPy with minimal code changes
- **Custom Kernels**: Allows easy creation and compilation of custom CUDA kernels for optimized operations
- **Applications**: Ideal for data science, machine learning, and scientific computing




https://cupy.dev/

# CuPy: GPU-Accelerated Python Library

**NumPy**

```
import numpy as np
size = 10000
A = np.random.rand(size, size)
B = np.random.rand(size, size)
C = np.dot(A, B)
```

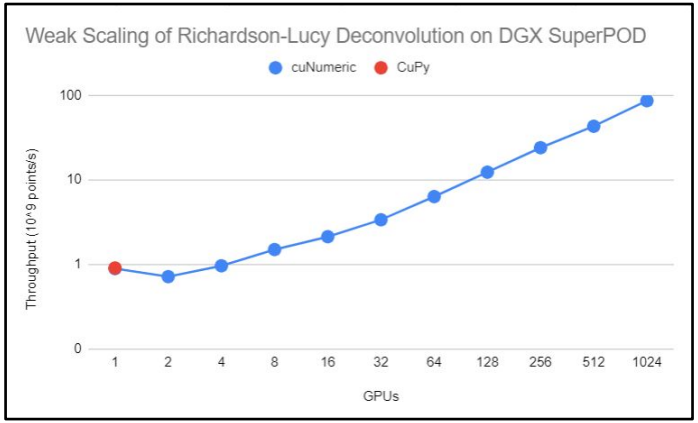
**CuPy**

```
import cupy as cp
size = 10000
A = cp.random.rand(size, size)
B = cp.random.rand(size, size)
C = cp.dot(A, B)
```

https://labs.icahn.mssm.edu/minervalab/wp-content/uploads/sites/342/2024/04/MountSinai_accelerated_general_data_science-compressed.pdf

# cuNumeric: GPU-Accelerated NumPy Replacement

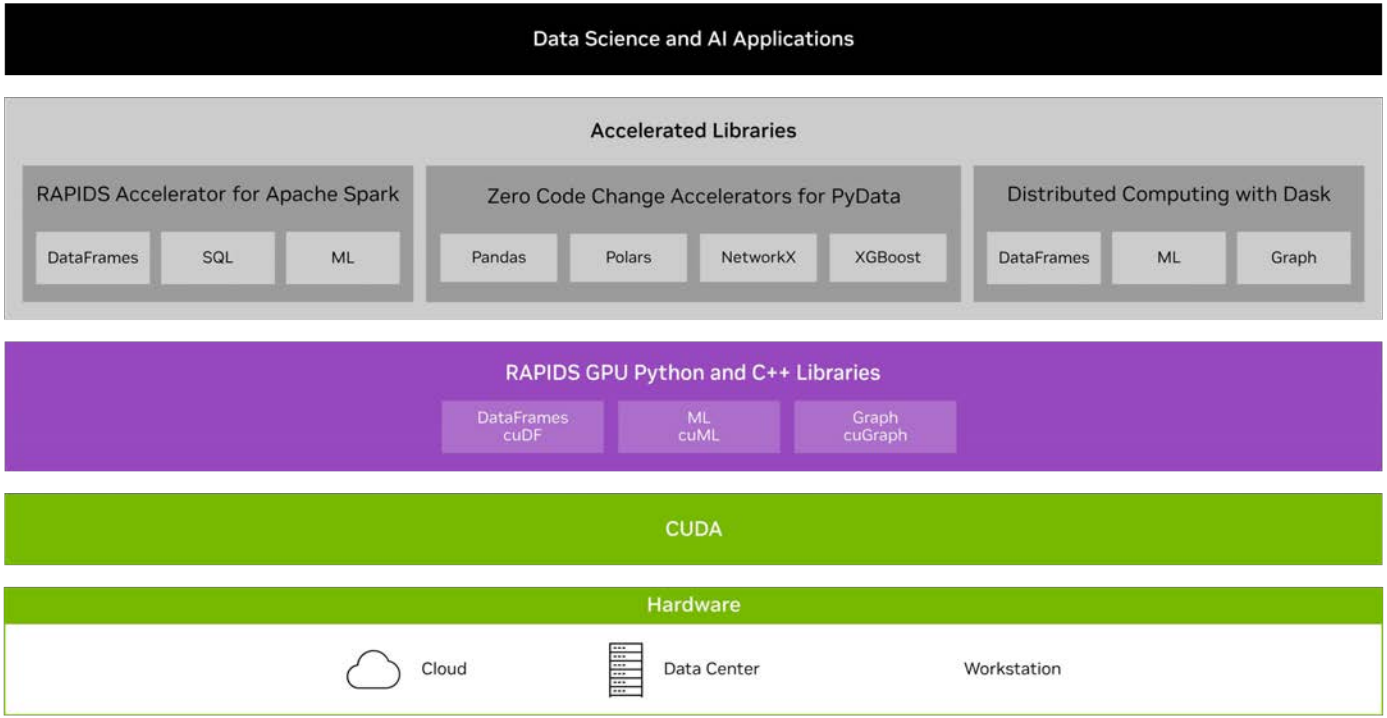
- **Overview**: cuNumeric is a drop-in replacement for NumPy, designed to scale computations across multiple GPUs and nodes without code changes.
- **Key Features**
  - Full NumPy functionality with GPU acceleration
  - Seamless integration with existing Python workflows
  - Leverages the Legate framework for distributed computing
- **Use Case**: Ideal for large-scale data processing tasks in scientific computing, machine learning, and AI
- **Benefit:** Significant performance gains in handling complex numerical computations on large clusters




https://developer.nvidia.com/cunumeric

# RAPIDS

- RAPIDS is a collection of open-source software libraries and APIs that enables you to run complete data science and analytics pipelines entirely on GPUs




https://developer.nvidia.com/rapids

# RAPIDS

| Category | CPU Libraries | GPU Libraries (RAPIDS) |
|---|---|---|
| Data Processing | Pandas | cuDF |
| Machine Learning | scikit-learn | cuML |
| Graph Processing | NetworkX | cuGraph |
| Geospatial Data | GeoPandas, SciPy | cuSpatial |
| Signal Processing | SciPy.signal | cuSignal |
| Image Processing | scikit-image | cuCIM |

# cuDF

- A GPU-accelerated DataFrame library
- Similar to pandas, but utilizes the power of GPUs for enhanced performance
- Part of the RAPIDS AI framework developed by NVIDIA
- Designed for large-scale data processing and analytics
- Installable via Conda or Pip

```
import cudf as pd
import numpy as np

# Load a CSV file as a cuDF DataFrame
data_gpu = pd.read_csv("data/sample_data.csv")

# Generate some statistics
mean_values = data_gpu.mean()
print("Mean of each column:\n", mean_values)

# Filtering rows based on a condition
filtered_data =
data_gpu[data_gpu['column_name'] > 50]

# Display filtered data
filtered_data.head(5)
```

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# CPU vs. GPU ETL Workflows

- **Time Consuming ETL (Extract, Transform, Load) Steps (CPU-Powered)**
  - **Configure ETL**: Requires extensive configuration and manual work.
  - **Data Download & Preparation**: Long hours waiting for data downloads
  - **Frequent Restarts**: Restart workflows due to errors or missed steps
  - **Training Delays**: Minimal time left for model training, mostly focusing on data preparation
- **Accelerated ETL and Training (GPU-Powered)**:
  - **Fast Configuration**: Rapid setup of ETL pipelines
  - **Optimized Data Handling**: Handles datasets with increased speed
  - **Integrated Validation and Training**: Time saved for comprehensive model training and validation
  - **Reduced Rework**: Minimized workflow restarts, leading to more efficient work cycles
- **Takeaway**: With GPU acceleration, data scientists spend significantly less time on repetitive ETL tasks, shifting their focus to training, testing, and optimizing machine learning models

# cuML - GPU Machine Learning Algorithms

| Category | Algorithm |
|---|---|
| **Clustering** | Density-Based Spatial Clustering of Applications with Noise (DBSCAN) |
| | Hierarchical Density-Based Spatial Clustering of Applications with Noise (HDBSCAN) |
| | K-Means |
| | Single-Linkage Agglomerative Clustering |
| **Dimensionality Reduction** | Principal Components Analysis (PCA) |
| | Incremental PCA |
| | Truncated Singular Value Decomposition (tSVD) |
| | Uniform Manifold Approximation and Projection (UMAP) |
| | Random Projection |

https://github.com/rapidsai/cuml

# cuML - GPU Machine Learning Algorithms

| Category | Algorithm |
|---|---|
| **Linear Models for Regression or Classification** | Linear Regression |
| | Linear Regression with Lasso or Ridge Regularization |
| | ElasticNet Regression |
| | LARS Regression |
| | Logistic Regression |
| | Naive Bayes |
| | Stochastic Gradient Descent (SGD), Coordinate Descent (CD), and Quasi-Newton (QN) (including L-BFGS and OWL-QN) solvers for linear models |

https://github.com/rapidsai/cuml

# cuML - GPU Machine Learning Algorithms

| Category | Algorithm |
|---|---|
| **Nonlinear Models for Regression or Classification** | Random Forest (RF) Classification |
| | Random Forest (RF) Regression |
| | Inference for decision tree-based models |
| | K-Nearest Neighbors (KNN) Classification |
| | K-Nearest Neighbors (KNN) Regression |
| | Support Vector Machine Classifier (SVC) |
| | Epsilon-Support Vector Regression (SVR) |

https://github.com/rapidsai/cuml

# cuML - GPU Machine Learning Algorithms

| Category | Algorithm |
|---|---|
| **Preprocessing** | Standardization, or mean removal and variance scaling / Normalization / Encoding categorical features / Discretization / Imputation of missing values / Polynomial features generation / and coming soon custom transformers and non-linear transformation |
| **Time Series** | Holt-Winters Exponential Smoothing |
| | Auto-regressive Integrated Moving Average (ARIMA) |
| **Model Explanation** | SHAP Kernel Explainer |
| | SHAP Permutation Explainer |

https://github.com/rapidsai/cuml

# Numba

- Numba is a just-in-time (JIT) compiler that translates Python code to machine code at runtime, significantly improving performance for numerical computations
- Key Features
  - **JIT Compilation:** Numba compiles Python functions at runtime for fast performance
  - **Easy Integration:** Works seamlessly with NumPy and pandas
  - **Decorator-Based:** Use the @jit decorator to accelerate Python functions without code changes
  - **Support for GPUs:** Numba can target NVIDIA GPUs for parallel computation (@cuda.jit)
- Benefits
  - **Speed:** Offers speed-ups comparable to compiled languages like C
  - **Ease of Use:** No need to rewrite Python code in C or other languages to get better performance
  - **Parallelization:** Enables easy parallel programming with features like GPU support

# Numba

## CPU

```
from numba import jit

@jit
def vector_add(a, b):
    n = len(a)
    result = np.zeros(n)
    for i in range(n):
        result[i] = a[i] + b[i]
    return result

# Vector addition on the CPU
result = vector_add(a, b)
```

## GPU

```
from numba import cuda

@cuda.jit
def vector_add_gpu(a, b, result):
    i = cuda.grid(1)
    if i < len(a):
        result[i] = a[i] + b[i]

# Define grid and block size
threads_per_block = 256
blocks_per_grid = (len(a) + (threads_per_block - 1))
// threads_per_block

# Launch kernel
vector_add_gpu[blocks_per_grid,
threads_per_block](a, b, result)
```

https://labs.icahn.mssm.edu/minervalab/wp-content/uploads/sites/342/2024/04/MountSinai_accelerated_general_data_science-compressed.pdf

# Medical Open Network for Artificial Intelligence (MONAI)

- Initiative by NVIDIA and King's College London
- Built to create an inclusive AI research community for healthcare imaging
- Collaboration includes academic and industry leaders
- Provides open-source PyTorch-based frameworks for:
  - Annotation, model building, training, deployment, and optimization
- Focus on reproducibility and collaboration
- Key components:
  - **MONAI Core:** Training AI models in healthcare imaging
  - **MONAI Label:** Smart image annotation
  - **MONAI Deploy SDK:** Convert models into deployable AI applications
  - **MONAI Model Zoo:** Pre-built medical imaging models

https://monai.io/

https://github.com/Project-MONAI

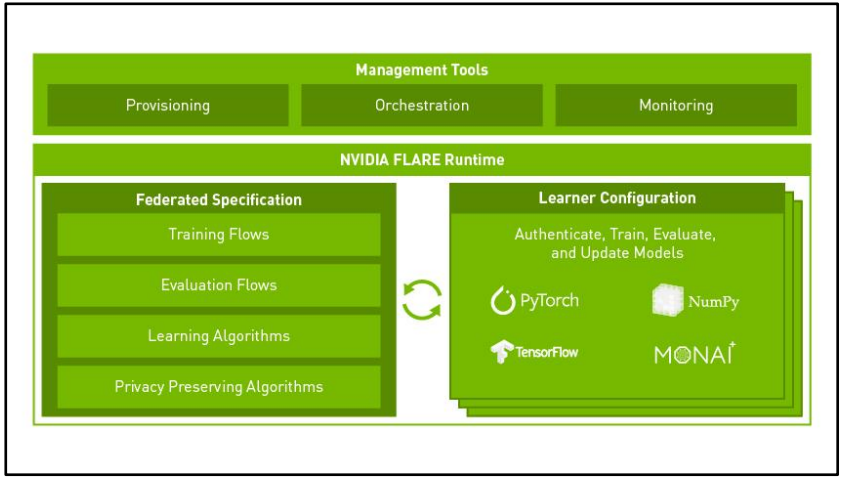
# NVIDIA Holoscan

- NVIDIA Holoscan is the sensor processing platform that streamlines the development and deployment of AI and high-performance computing (HPC) applications for real-time insights
- **Key Benefits**
  - **Sensor Processing**: Supports video capture, ultrasound research, and legacy medical devices
  - **Low Latency**: Holoscan SDK helps measure end-to-end latency for video processing
  - **AI Pipelines:** Access AI reference pipelines for radar, high-energy light sources, endoscopy, ultrasound, and other streaming video applications
- **Use Cases**
  - **Medical Devices**: Real-time AI for surgery, helping clinical teams with patient-specific decisions
  - **Edge Computing**: Scalable AI solutions from surgery to satellites

https://www.nvidia.com/en-us/clara/holoscan/

# NVIDIA FLARE

- NVIDIA FLARE (NVIDIA Federated Learning Application Runtime Environment) is a domain-agnostic, open-source, and extensible SDK for Federated Learning
- **Key Features**:
  - **Privacy-Preserving Algorithms**: Protects data privacy with algorithms that prevent reverse engineering of model updates
  - **Distributed Multi-Party Collaboration**: Enables AI model development across diverse data sources without sharing data
  - **Supports Popular ML/DL Frameworks**: Integrates seamlessly with frameworks like PyTorch, TensorFlow, and more
  - **Extensible Management Tools**: Offers SSL certifications, admin console, and TensorBoard for experiment monitoring




https://developer.nvidia.com/flare

# Ways to Accelerate with GPUs: OpenACC Directives

# OpenACC Directives

- OpenACC is a directive-based programming model for parallel computing, designed to make performance-portable code accessible to scientists and engineers across various HPC hardware platforms. It enables efficient parallelization without the complexities of low-level programming
- Key Benefits:
  - **Simplified Code Parallelism:** Use directives to easily identify parallel regions
  - **Accelerator Ready:** Ideal for many-core GPUs and multicore CPUs
  - **Less Effort:** Reduces development time and complexity compared to CUDA or OpenCL

**C**

```
#pragma acc directive [clause [,] clause] ...
{
// Code to be executed in parallel
}
```

**Fortran**

```
!$acc directive [clause [,] clause] ...
! Code to be executed in parallel
!$acc end directive
```

https://labs.icahn.mssm.edu/minervalab/wp-content/uploads/sites/342/2024/05/FiveWays-HealthCare-April2024.pdf

# SAXPY Example: SAXPY is “Single-Precision A times X Plus Y”

## SAXPY in C

```
void saxpy_with_offset(int n, float a,
float *x, float *restrict y, int offset)
{
 #pragma acc kernels
  for (int i = offset; i < n + offset; ++i)
  {
    y[i] = a * x[i - offset] + y[i];
  }
}

...

// Perform SAXPY on 1M elements with an
offset of 1000
saxpy_with_offset(1 << 20, 2.5, x, y,
1000);
...
```

## SAXPY in Fortran

```
subroutine saxpy_with_offset(n, a, x, y,
offset)
    real :: x(:), y(:), a
    integer :: n, i, offset

    !$acc kernels
    do i = offset + 1, n + offset
        y(i) = a * x(i - offset) + y(i)
    end do
    !$acc end kernels

end subroutine saxpy_with_offset

...

! Perform SAXPY on 1M elements with an offset
of 1000
call saxpy_with_offset(2**20, 2.5, x, y, 1000)
...
```

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# Ways to Accelerate with GPUs: CUDA Programming

# CUDA Programming

- What is CUDA?
  - CUDA (Compute Unified Device Architecture) is a parallel computing platform and programming model developed by NVIDIA
  - It enables developers to utilize the power of NVIDIA GPUs for general-purpose computing
- Key Features:
  - **Parallel Computing**: CUDA allows thousands of threads to execute concurrently, maximizing the utilization of the GPU.
  - **Heterogeneous Programming**: Code can run on both the CPU (host) and GPU (device), allowing for efficient division of tasks.
  - **Flexible Memory Management**: CUDA provides various types of memory (global, shared, constant) that can be optimized for different tasks.
- CUDA provides APIs for C/C++, Fortran, Python, Julia
- CUDA-aware MPI implementations include OpenMPI, MVAPICH, Spectrum MPI, and others

# CUDA C

```
void saxpy_offset_serial(int n, float a,
float *x, float *y, int offset)
{
    for (int i = offset; i < n + offset;
++i)
    {
        y[i] = a * x[i - offset] + y[i];
    }
}

// Perform SAXPY on 1M elements with an
offset of 1000
saxpy_offset_serial(4096 * 256, 2.0, x, y,
1000);
```

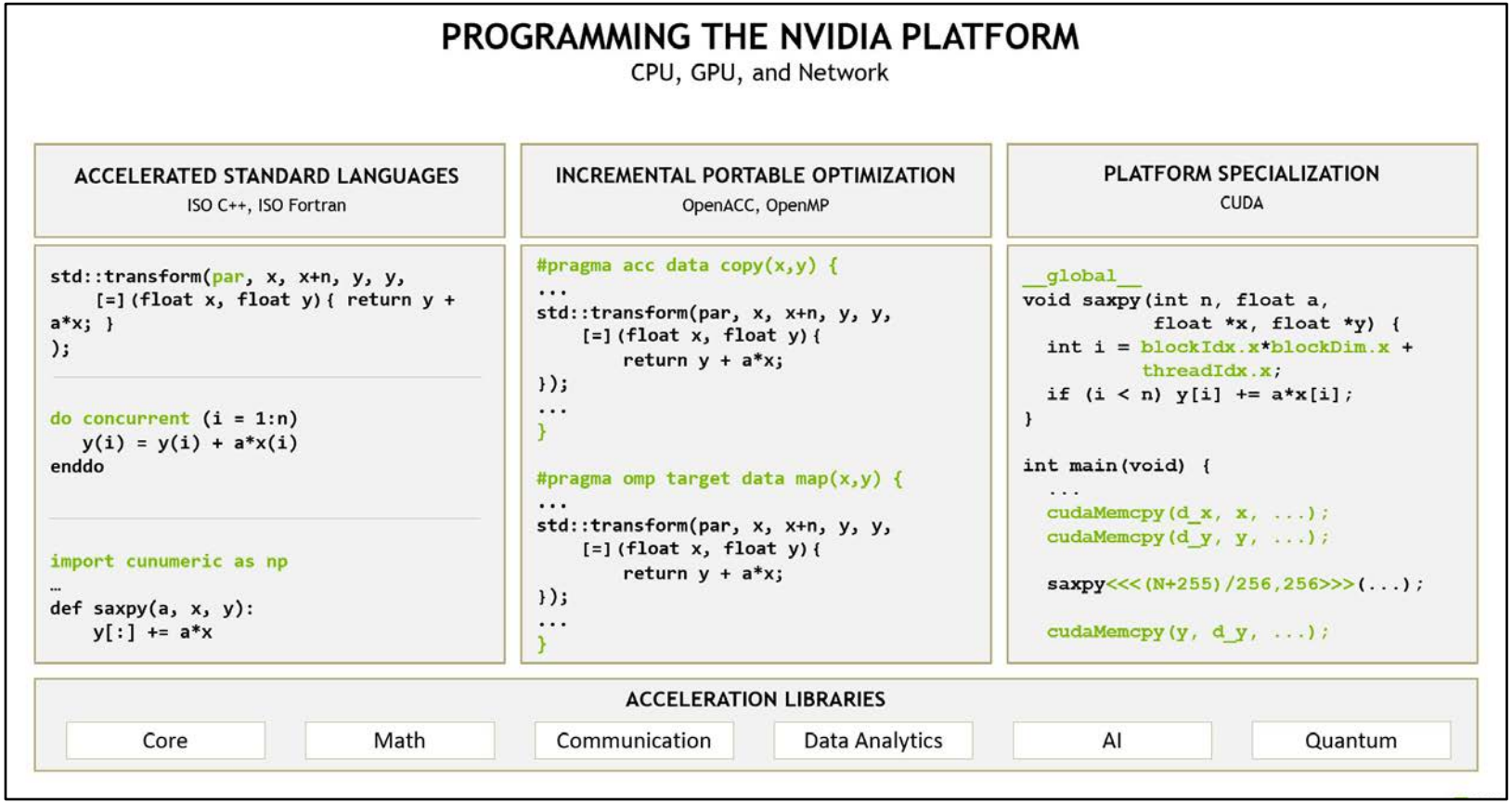
```
__global__
void saxpy_offset_parallel(int n, float a,
float *x, float *y, int offset)
{
    int i = blockIdx.x * blockDim.x +
threadIdx.x + offset;
    if (i < n + offset) {
        y[i] = a * x[i - offset] + y[i];
    }
}

// Perform SAXPY on 1M elements with an
offset of 1000
saxpy_offset_parallel<<<4096, 256>>>(n,
2.0, x, y, 1000);
```

https://labs.icahn.mssm.edu/minervalab/wp-content/uploads/sites/342/2024/05/FiveWays-HealthCare-April2024.pdf

# Ways to Accelerate with GPUs: Standard Language Parallelism

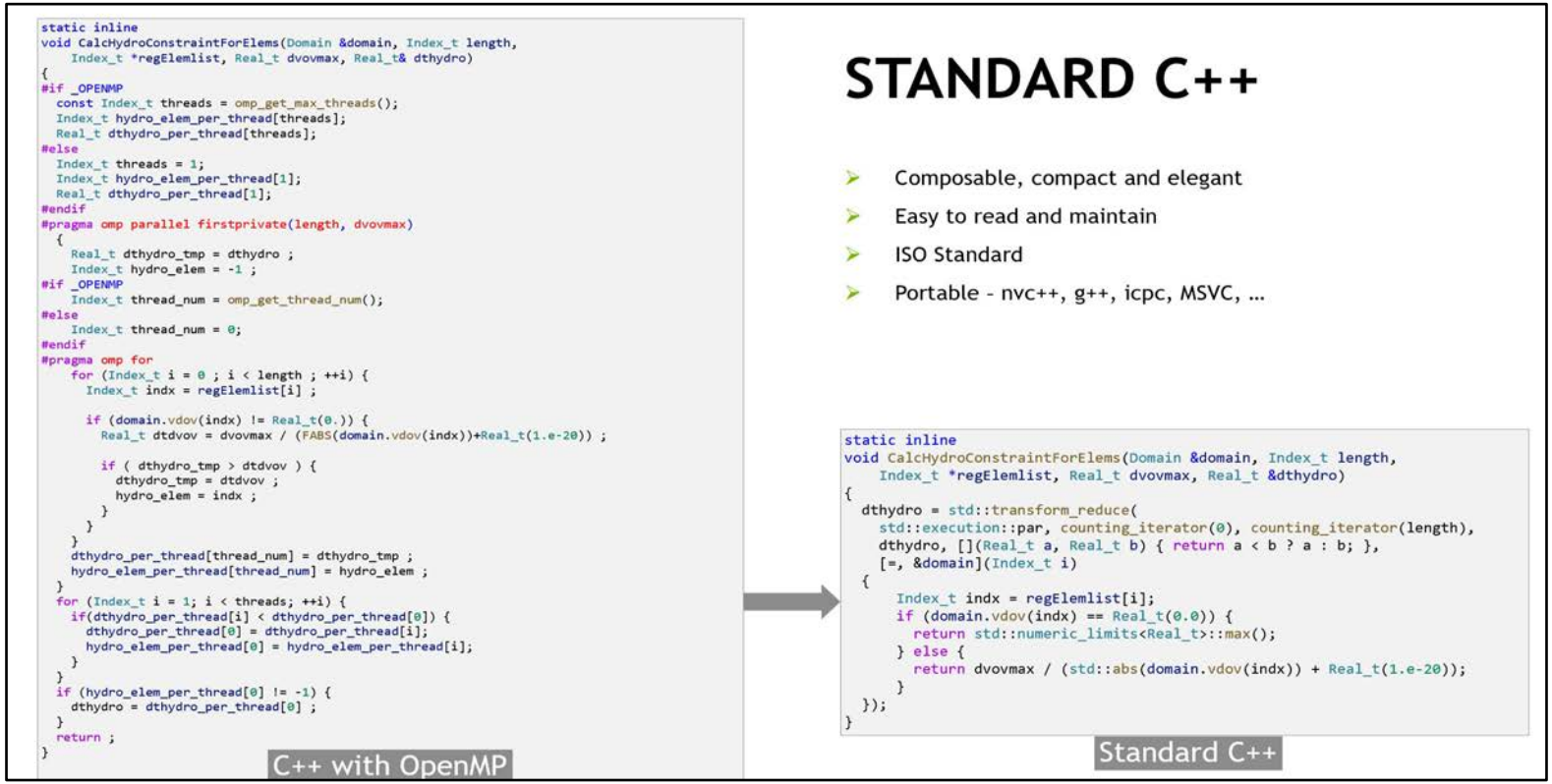
# Standard Language Programming




https://developer-blogs.nvidia.com/wp-content/uploads/2022/01/Fig-1-Programming-the-Nvidia-Platform-2.png

# Standard Language Programming

## Lulesh Hydronynamics Mini-app




https://developer-blogs.nvidia.com/wp-content/uploads/2022/01/Fig-2-Standard-C-1.png

# User GPU Software Environment - Major packages

**OS:** **Rocky 9.4** with **glibc-2.34(GNU C library) available**

- Packages with GPU support:
  - Schrödinger Suite, Amber tools, NAMD, Gromacs, Alpha Fold2, etc.
- AI tools with python/3.12.5
  - CuPy, cuDF, cuML, Numba, scikit-learn, Scanpy, Squidpy, etc.
  - Minerva Python instruction
- AI tools with conda
  - MONAI, Rapids, NVFlare, tensorflow, pytorch, etc.
  - Minerva conda instruction
- AI tools with singularity
  - Holoscan, BioNeMo, Parabricks, DeepVariant, etc.
  - Minerva singularity instruction
  - Minerva Singularity training
- Cuda toolkit versions up to 12.4.0
- Nsight Systems

# Important Reminder

- Need assistance? Feel free to contact us at:

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