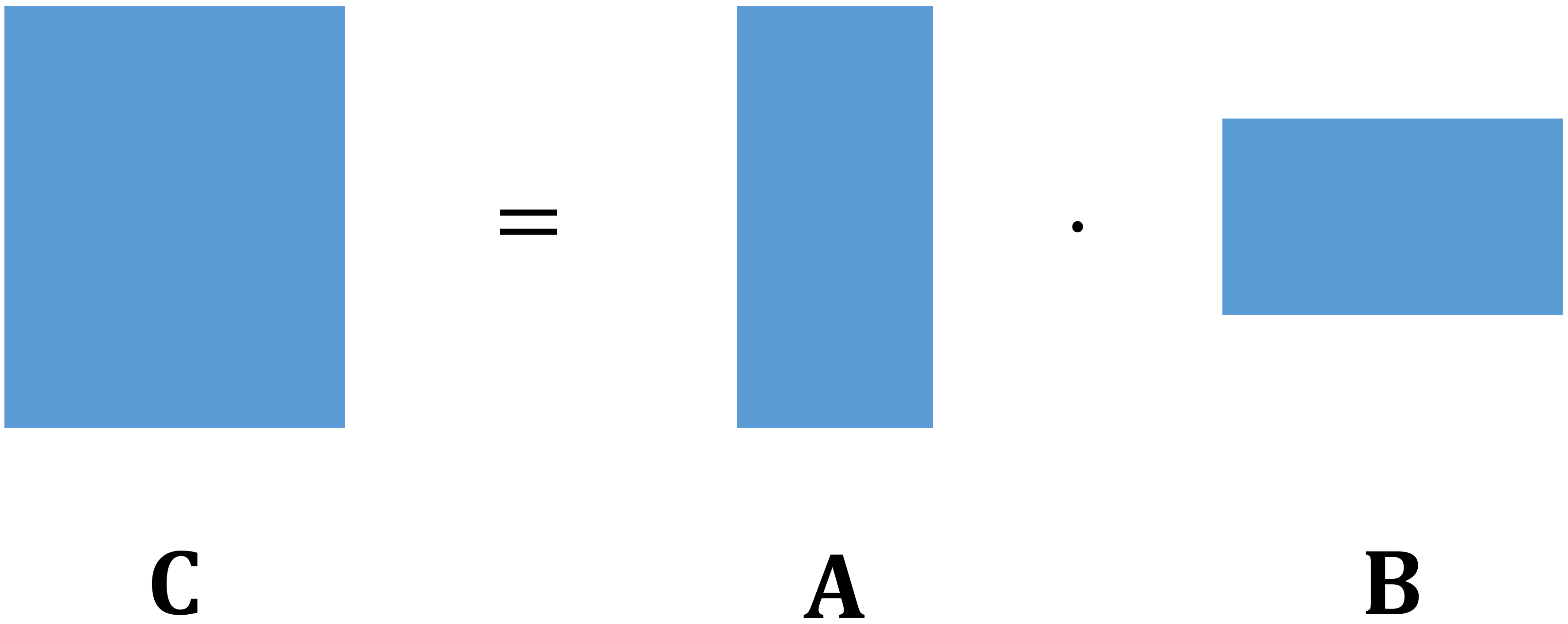
Scientific Computing Libraries

Xuting Tang

Matrix Multiplication

Task: Given $\mathbf{A} \in \mathbb{R}^{m \times n}$ and $\mathbf{B} \in \mathbb{R}^{n \times p}$, compute $\mathbf{C} = \mathbf{AB} \in \mathbb{R}^{m \times p}$.



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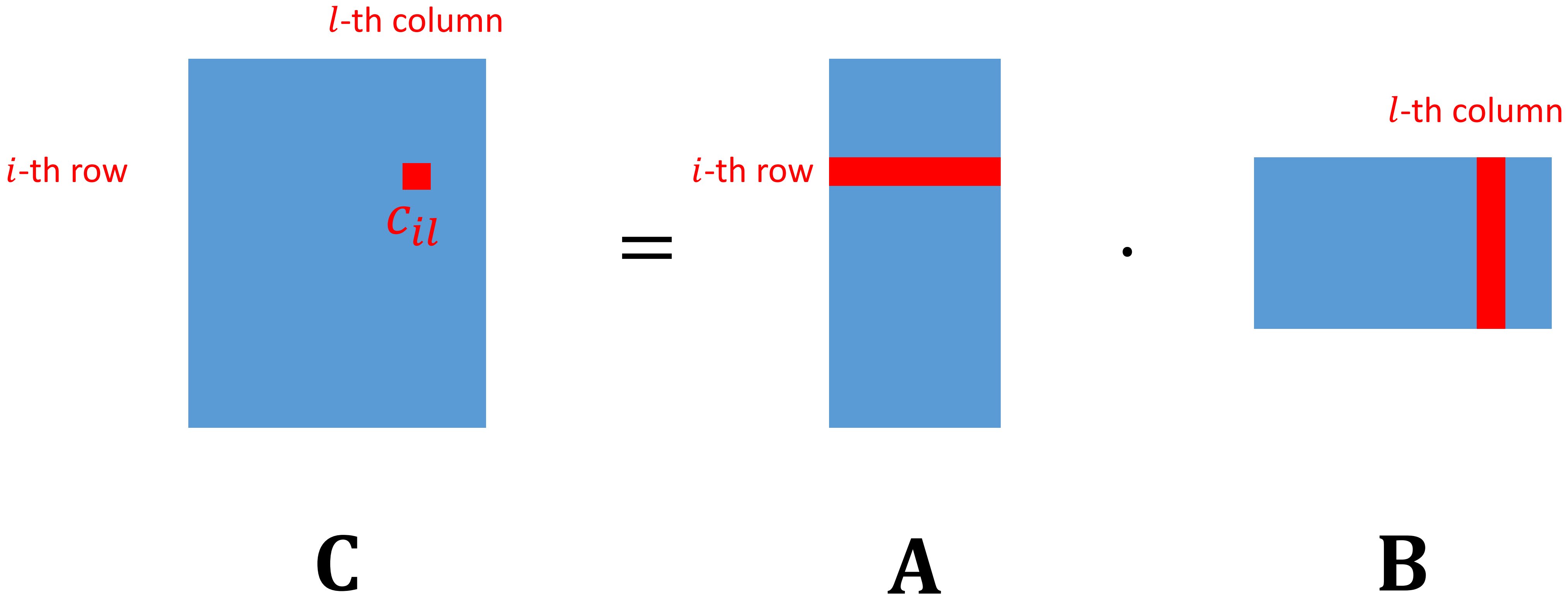

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```
C = numpy.zeros((m, p))
for i in range(m):
    for j in range(p):
        for l in range(n):
            C[i, j] += A[i, l] * B[l, j]
```

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- Suppose you have only **vector-vector multiplication** libraries.

```
C = numpy.zeros((m, p))
for i in range(m):
    for l in range(p):
        C[i, l] = numpy.dot(A[i, :], B[:, l])
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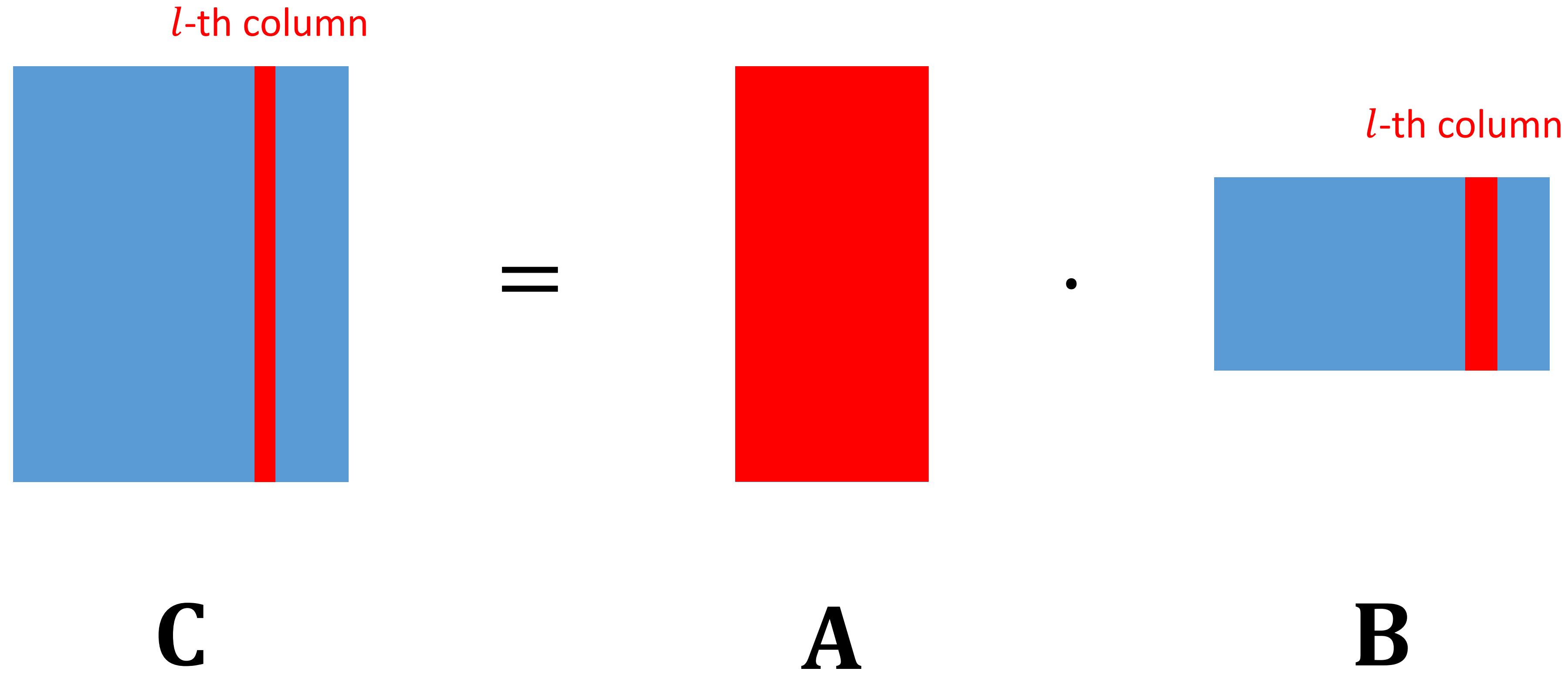
- Suppose you have **matrix-vector multiplication** libraries.



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- Suppose you have **matrix-matrix multiplication** libraries.

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- Which is the most efficient?
  - 3-level loop of **scalar multiplication**.
  - 2-level loop of **vector-vector multiplication**.
  - 1-level loop of **matrix-vector multiplication**.
  - Directly use **matrix-matrix multiplication** library.

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- Is your answer the same if the programming language is C or Fortran?

Basic Linear Algebra Subprograms (BLAS)

- **BLAS**: a library of standard building blocks for performing basic vector and matrix operations
- **Level 1 BLAS** perform scalar, vector, and vector-vector operations.
  - E.g., $\mathbf{y} \leftarrow \alpha\mathbf{x} + \mathbf{y}$, $a \leftarrow \mathbf{x}^T\mathbf{y}$, and $b \leftarrow \left|\left|\mathbf{x}\right|\right|_2$.
- **Level 2 BLAS** perform matrix-vector operations.
  - E.g, $\mathbf{y} \leftarrow \alpha\mathbf{A}\mathbf{x} + \beta\mathbf{y}$ and $\mathbf{A} \leftarrow \alpha\mathbf{x}\mathbf{y}^T + \mathbf{A}$.
- **Level 3 BLAS** perform matrix-matrix operations.
  - E.g, $\mathbf{A} \leftarrow \mathbf{A}^T$, $\mathbf{C} \leftarrow \mathbf{A}\mathbf{A}^T$, and $\mathbf{C} \leftarrow \alpha\mathbf{A}\mathbf{B} + \beta\mathbf{C}$.

Implementations of BLAS

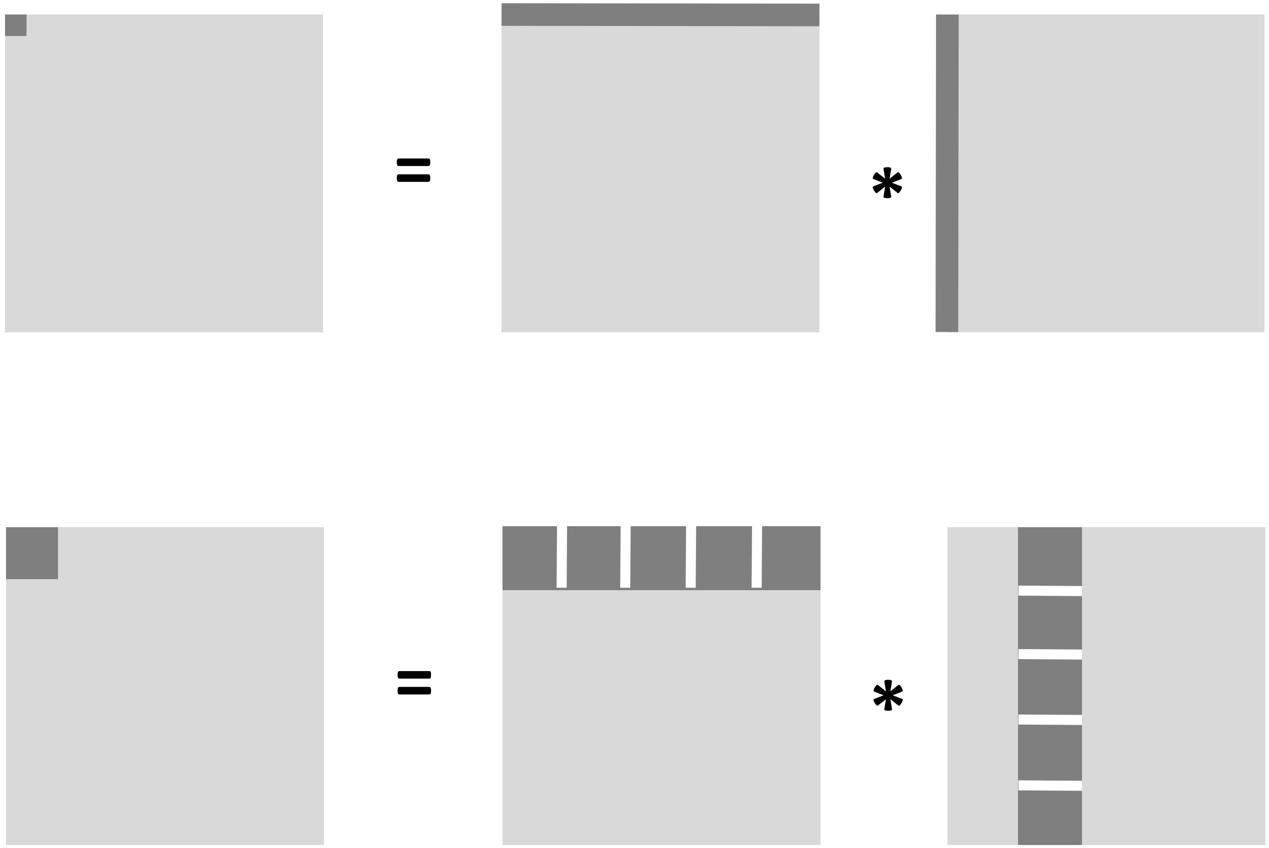
- **Netlib BLAS**: The **official** reference implementation, written in Fortran.

- **Intel MKL**: optimizations for Intel CPUs.
- **NVIDIA cuBLAS**: A fast GPU-accelerated implementation.
- **Accelerate**: Apple's framework for MacOS and iOS.

$\vdots$

Why are BLAS Fast?

- Efficient algorithms, e.g., blocking, to reduce time complexity.



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- Cache optimization by, e.g., spatial locality.
- Optimized for CPUs/GPUs, e.g.,
  - Intel MKL,
  - NVIDIA cuBLAS

Linear Algebra Package (LAPACK)

- LAPACK provides routines for numerical linear algebra, e.g.,
  - solving least squares $\min_{\mathbf{w}} \left|\left|\mathbf{X}\mathbf{w} - \mathbf{y}\right|\right|_2^2$,
  - eigenvalue problems $\mathbf{A} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^T$,
  - SVD $\mathbf{X} = \mathbf{U}\mathbf{\Lambda}\mathbf{V}^T$,
  - etc.

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  - etc.
- LAPACK uses Level 3 BLAS as much as possible.
- Numpy uses BLAS and LAPACK for matrix computation.
  - Numpy links against different BLAS on different machines.
  - Check your libraries: `numpy.__config__.show()`