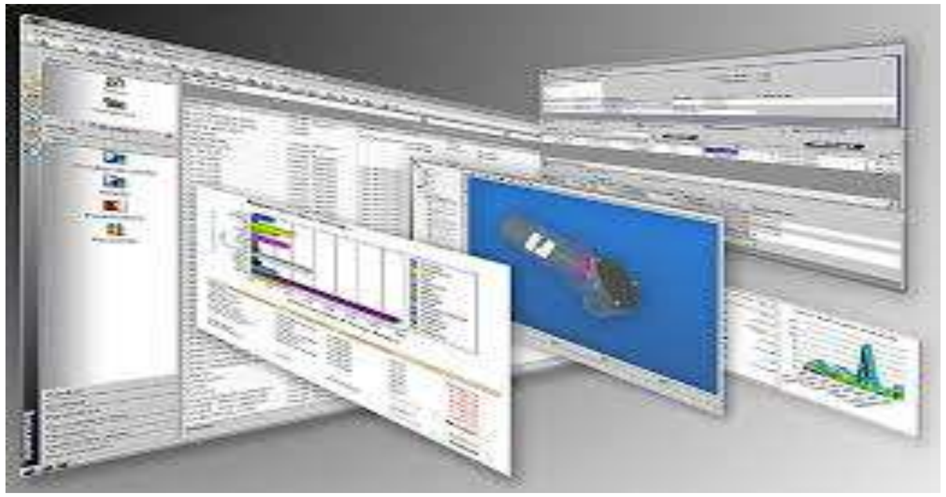
VORTECH BV
THE SCIENTIFIC SOFTWARE ENGINEERS

"LINC"
learning about interacting networks in climate

Hisham Ihshaish

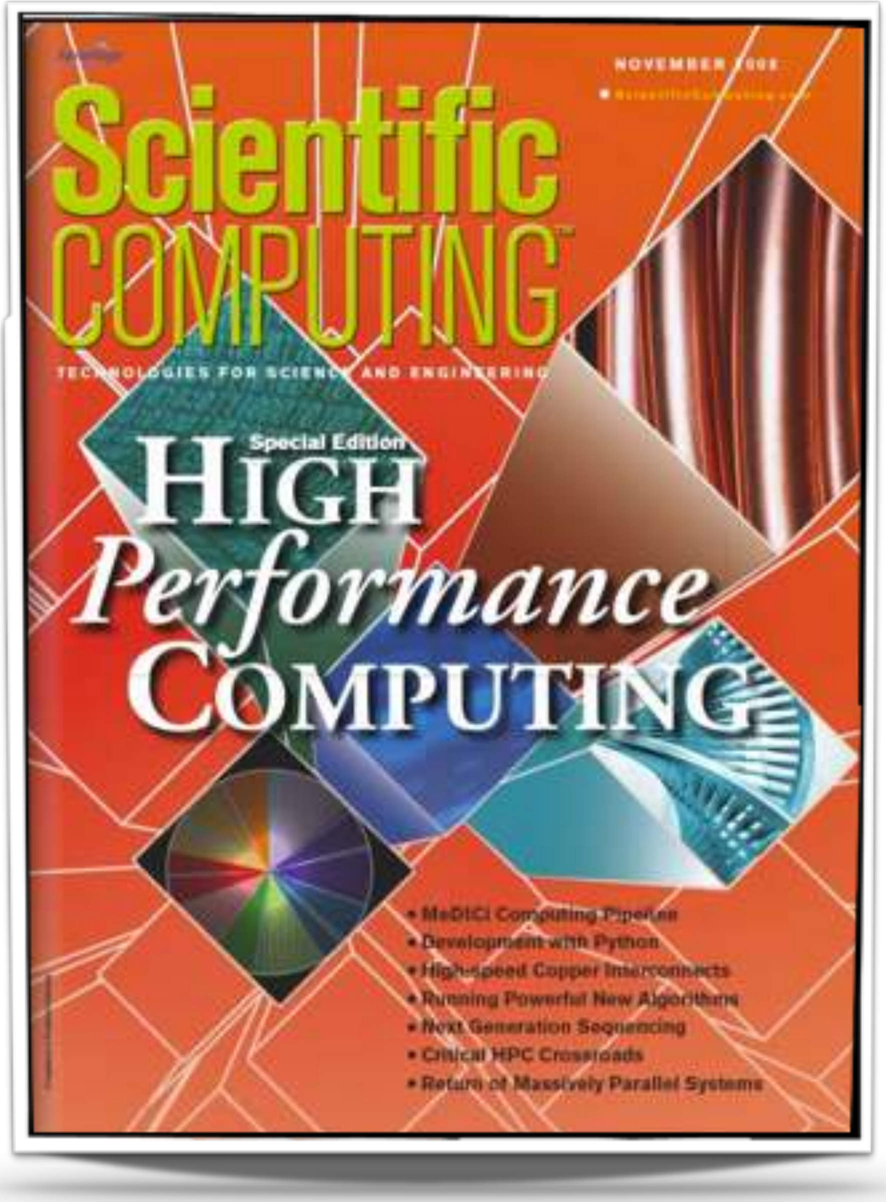
Parallel Software Tools for the Construction and Analysis of Complex Networks



LINC Workshop 4 – Montevideo
24-26/March/2014

Outline

- Introduction
- Computational challenges
- Parallel Software tools
    - Network construction
    - Network analysis
- Software architecture
- Usage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Scientific
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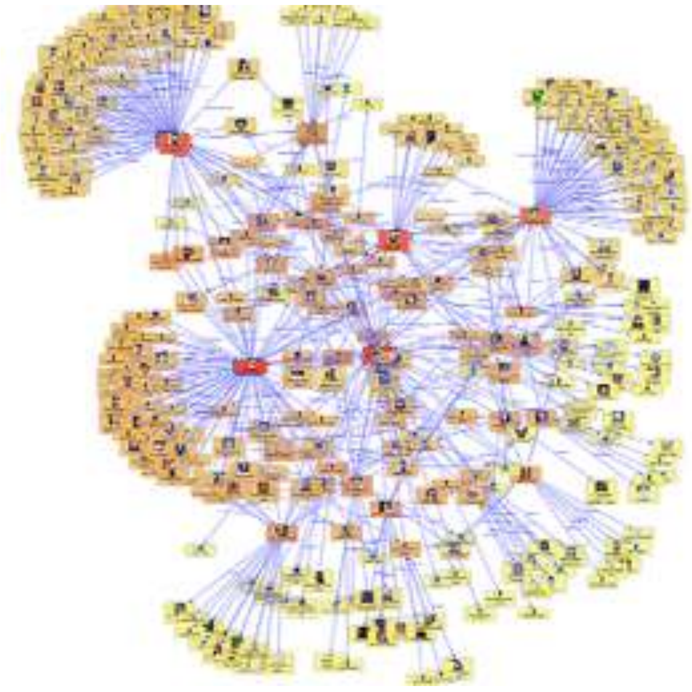
• MeDICi Computing Pipeline
• Development with Python
• High-speed Copper Interconnects
• Running Powerful New Algorithms
• Next Generation Sequencing
• Critical HPC Crossroads
• Return of Massively Parallel Systems

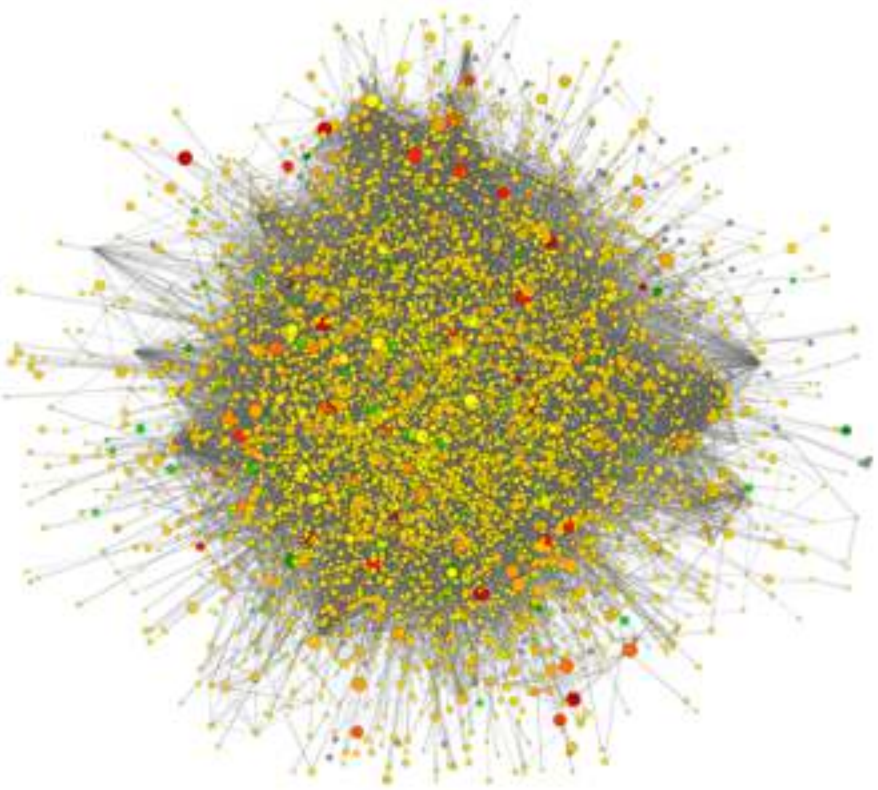
Introduction – large-scale data analysis

Social Networks



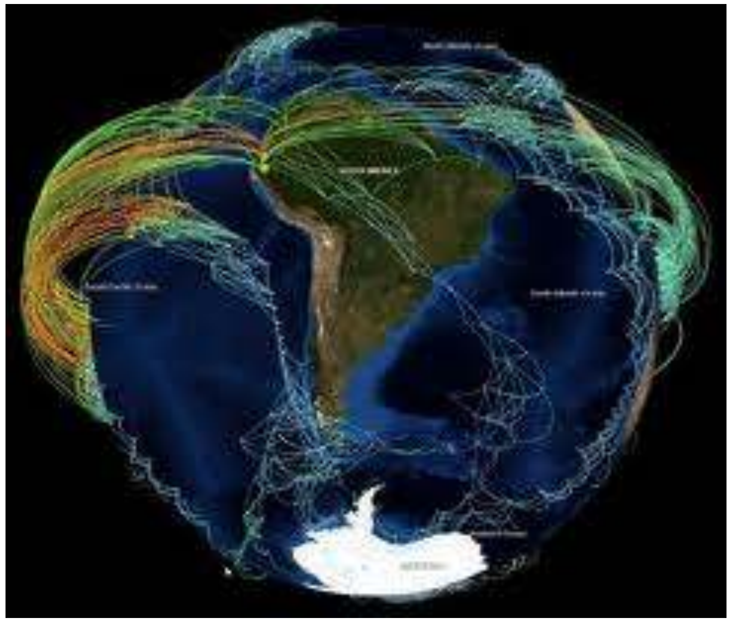
Application: e.g., identifying communities, information spread modeling

Bioinformatics



Application: e.g., identifying drug target proteins

Climate

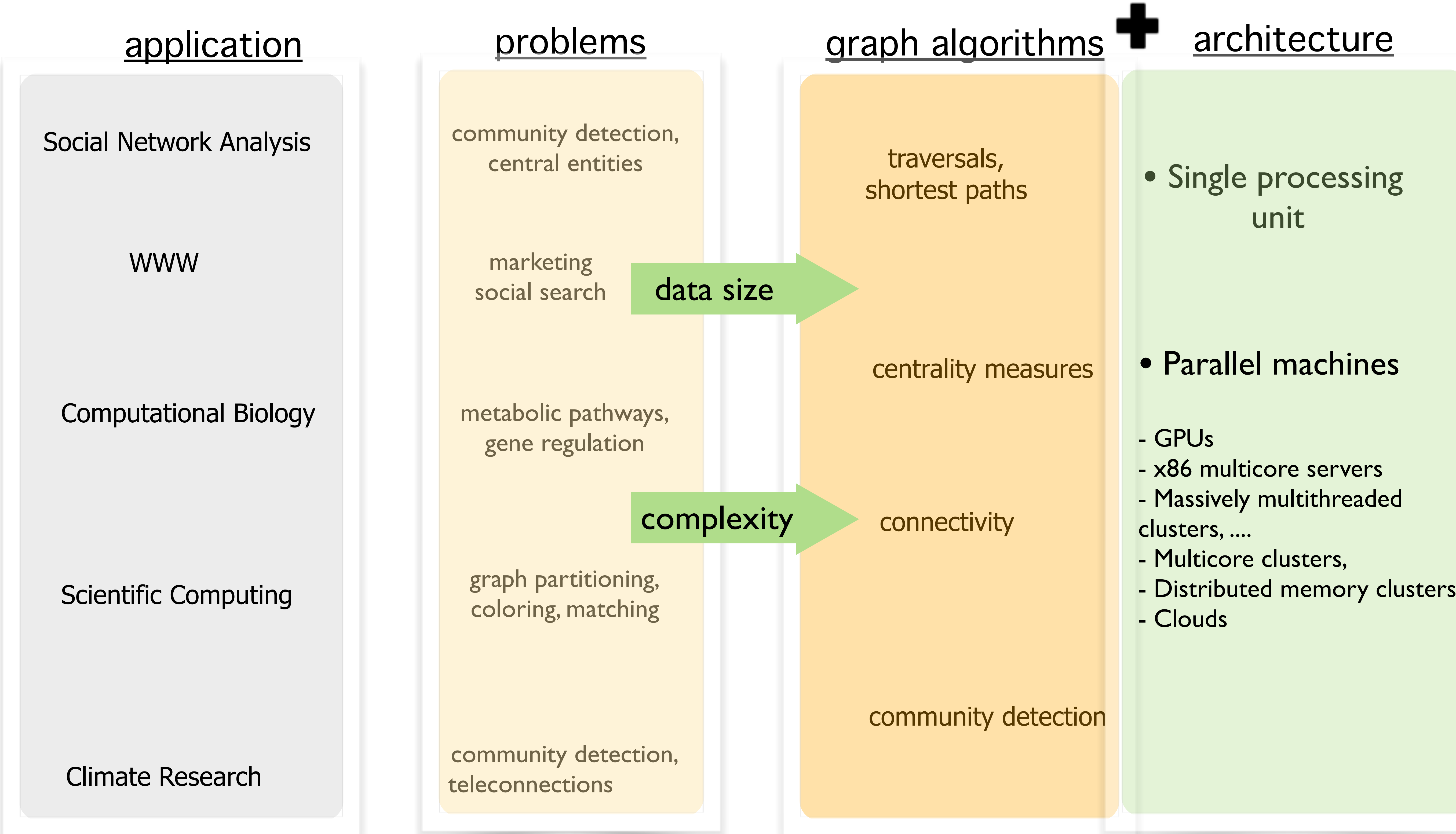


Application: e.g., identify patterns? analyze spatio-temporal interaction of climate variables

➡ **Sources of data:** simulations, experimental devices, the Internet, sensor networks

➡ **Challenges:** data size, heterogeneity, uncertainty, data quality, computational time

Introduction – from domain-specific to computation



application

Social Network Analysis

WWW

Computational Biology

Scientific Computing

Climate Research

problems

community detection, central entities

marketing social search

metabolic pathways, gene regulation

graph partitioning, coloring, matching

community detection, teleconnections

data size

complexity

graph algorithms

traversals, shortest paths

centrality measures

connectivity

community detection

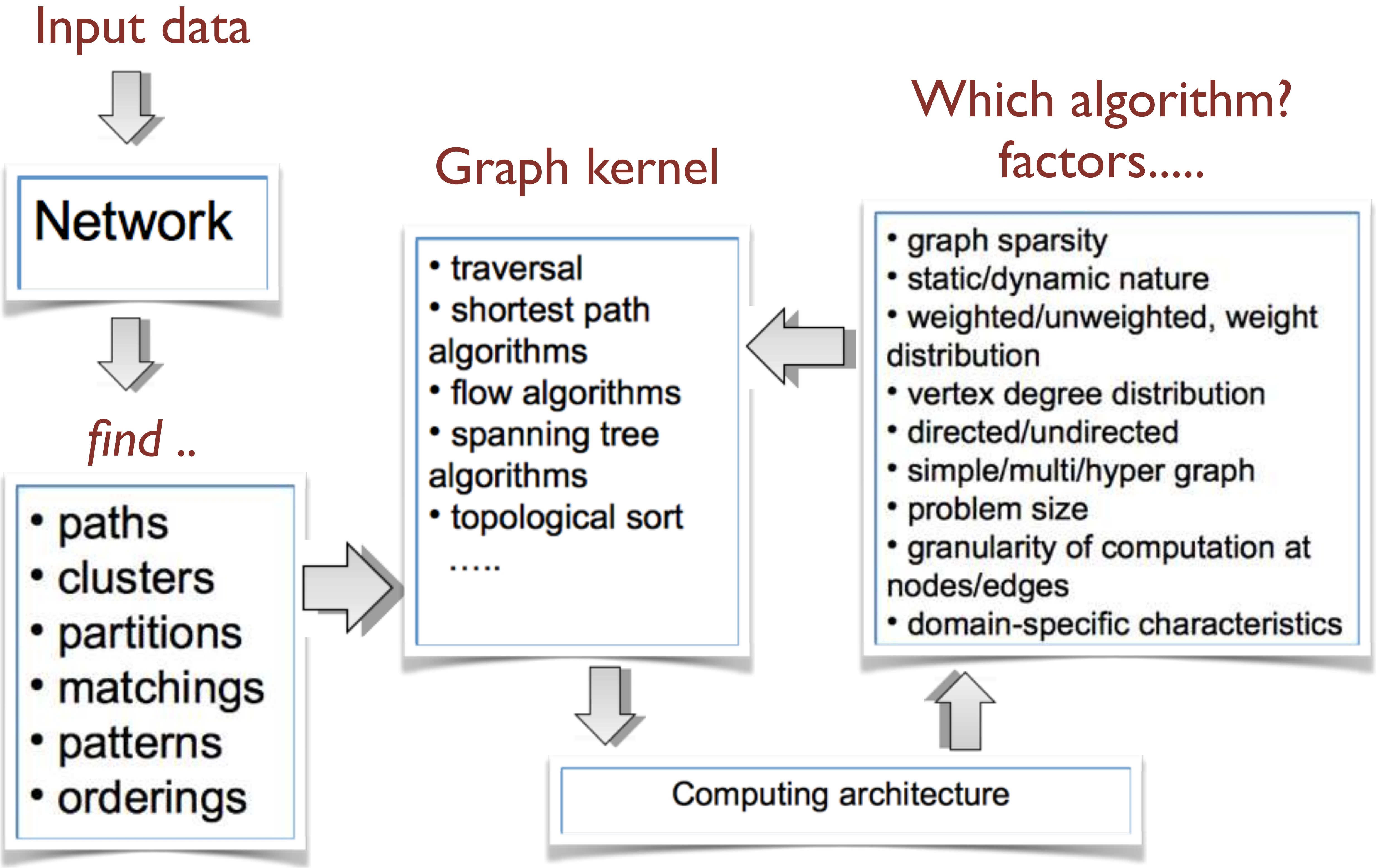
✚

architecture

- Single processing unit
- Parallel machines

- GPUs
- x86 multicore servers
- Massively multithreaded clusters, ….
- Multicore clusters,
- Distributed memory clusters
- Clouds

Introduction – from domain-specific to computation



Input data

Network

find ..

- paths
- clusters
- partitions
- matchings
- patterns
- orderings

Graph kernel

- traversal
- shortest path algorithms
- flow algorithms
- spanning tree algorithms
- topological sort

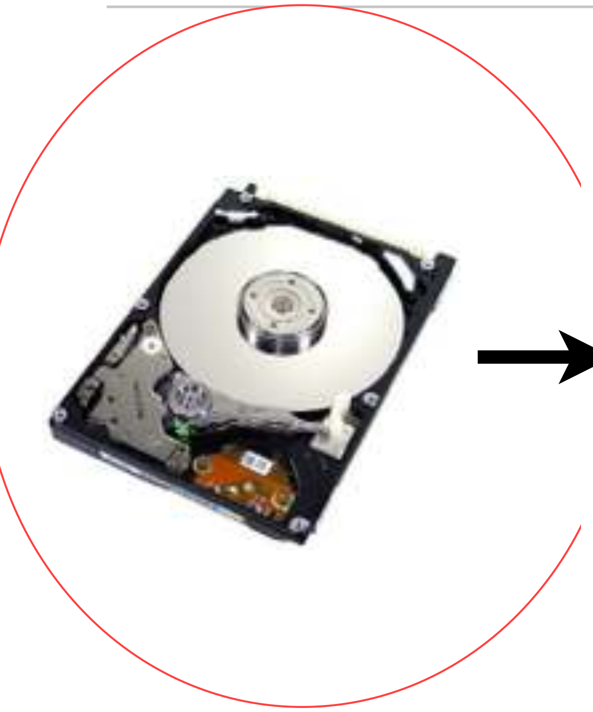
.....

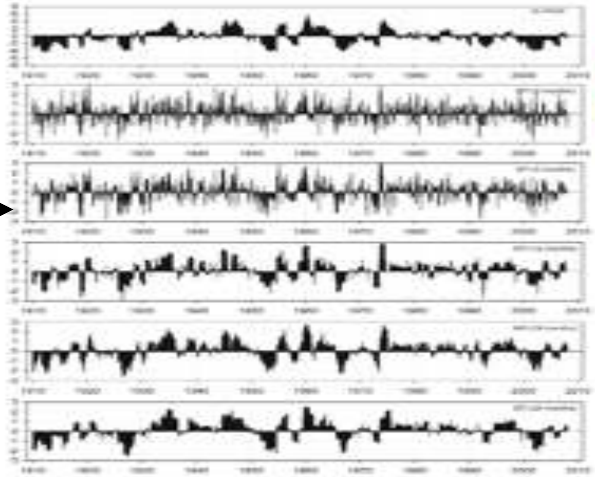
Which algorithm? factors.....

- graph sparsity
- static/dynamic nature
- weighted/unweighted, weight distribution
- vertex degree distribution
- directed/undirected
- simple/multi/hyper graph
- problem size
- granularity of computation at nodes/edges
- domain-specific characteristics

Computing architecture

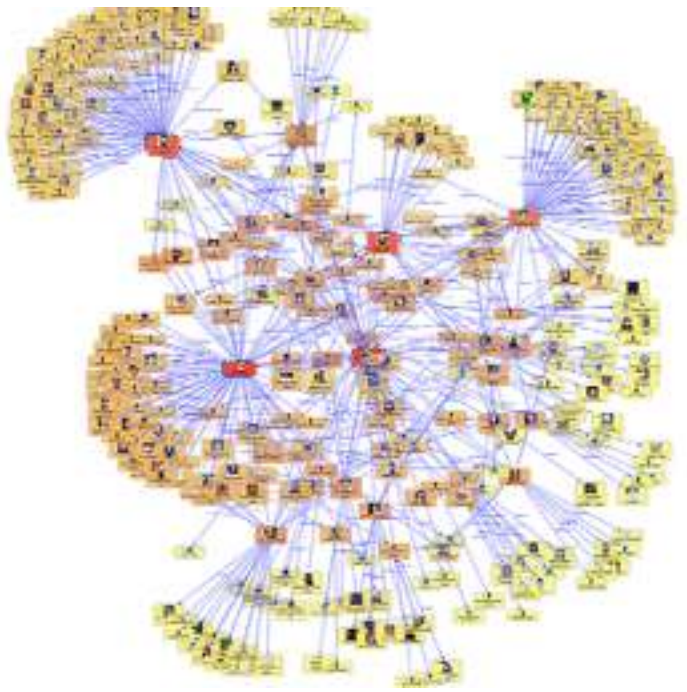
Introduction – computational challenges





1	0.01	0.41	0.922	0.01	0.41
0.01	1	.4.3	0.01	0.9	0.43
0.41	0.92	1	0.41	0.92	0.92
0.922	0.01	0.41	1	0.01	0.41
0.01	0.9	0.43	0.01	1	.4.3
0.41	0.92	0.92	0.41	0.92	1

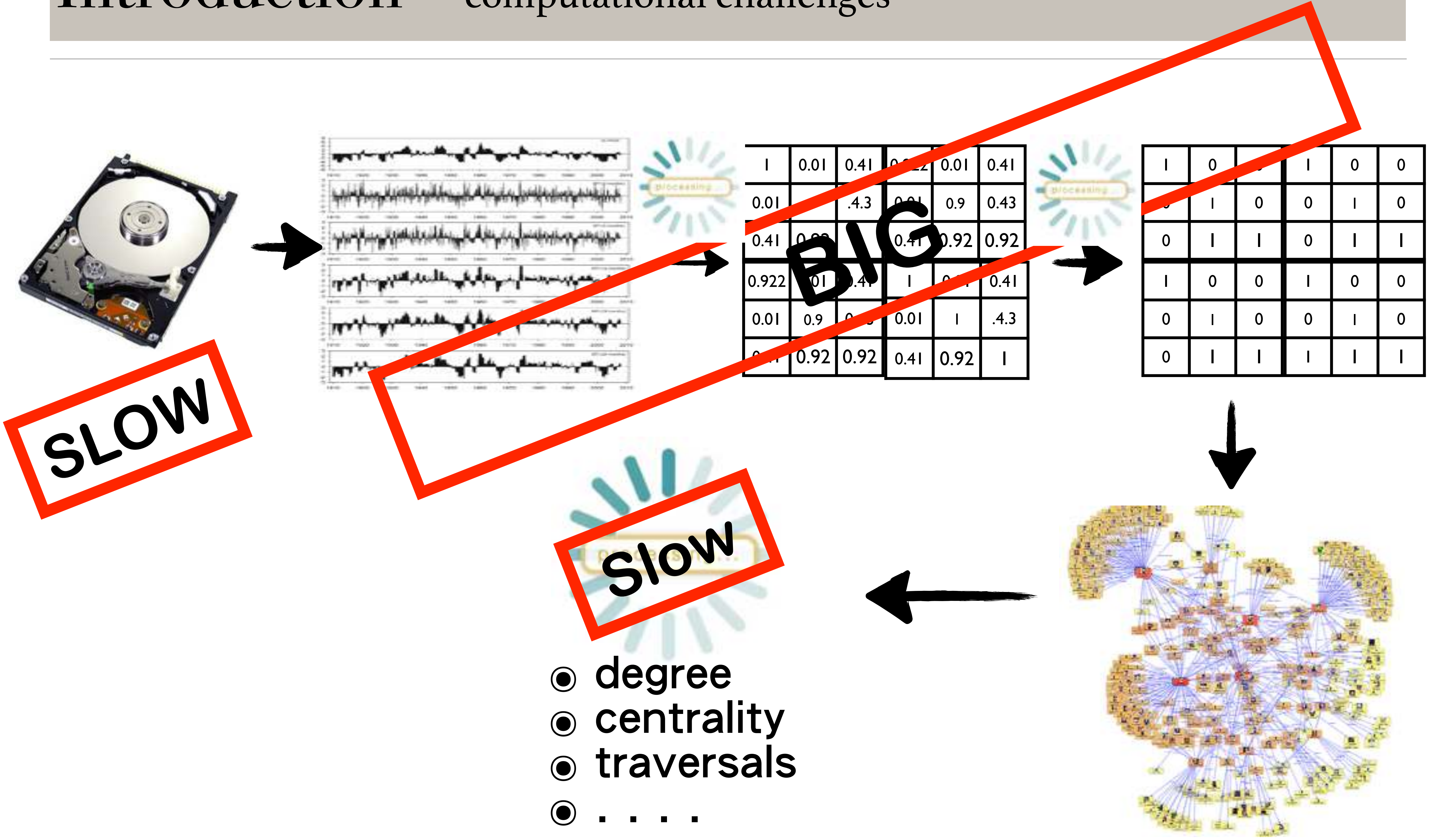
1	0	0	1	0	0
0	1	0	0	1	0
0	1	1	0	1	1
1	0	0	1	0	0
0	1	0	0	1	0
0	1	1	1	1	1



- ◉ degree
- ◉ centrality
- ◉ traversals
- ◉ . . . .

Hard “drive”

Introduction – computational challenges



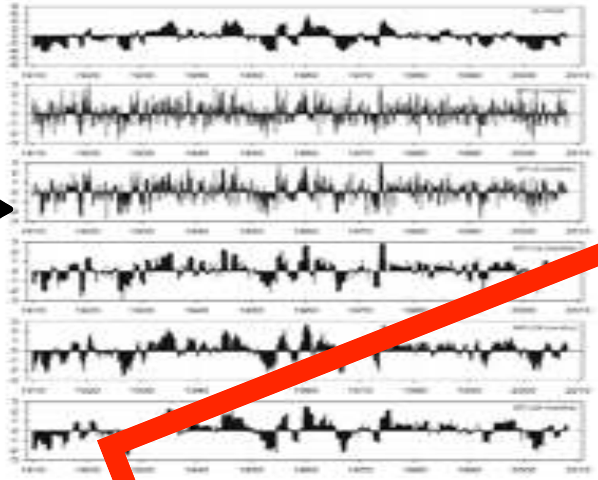
1	0.01	0.41	[illegible]	0.01	0.41
0.01	[illegible]	.4.3	[illegible]	0.9	0.43
0.41	[illegible]	[illegible]	[illegible]	0.92	0.92
0.922	[illegible]	[illegible]	1	[illegible]	0.41
0.01	0.9	[illegible]	0.01	1	.4.3
[illegible]	0.92	0.92	0.41	0.92	1

1	0	[illegible]	1	0	0
[illegible]	1	0	0	1	0
0	1	1	0	1	1
1	0	0	1	0	0
0	1	0	0	1	0
0	1	1	1	1	1

- degree
- centrality
- traversals
- . . . .

Introduction – computational challenges

SLOW



BIG

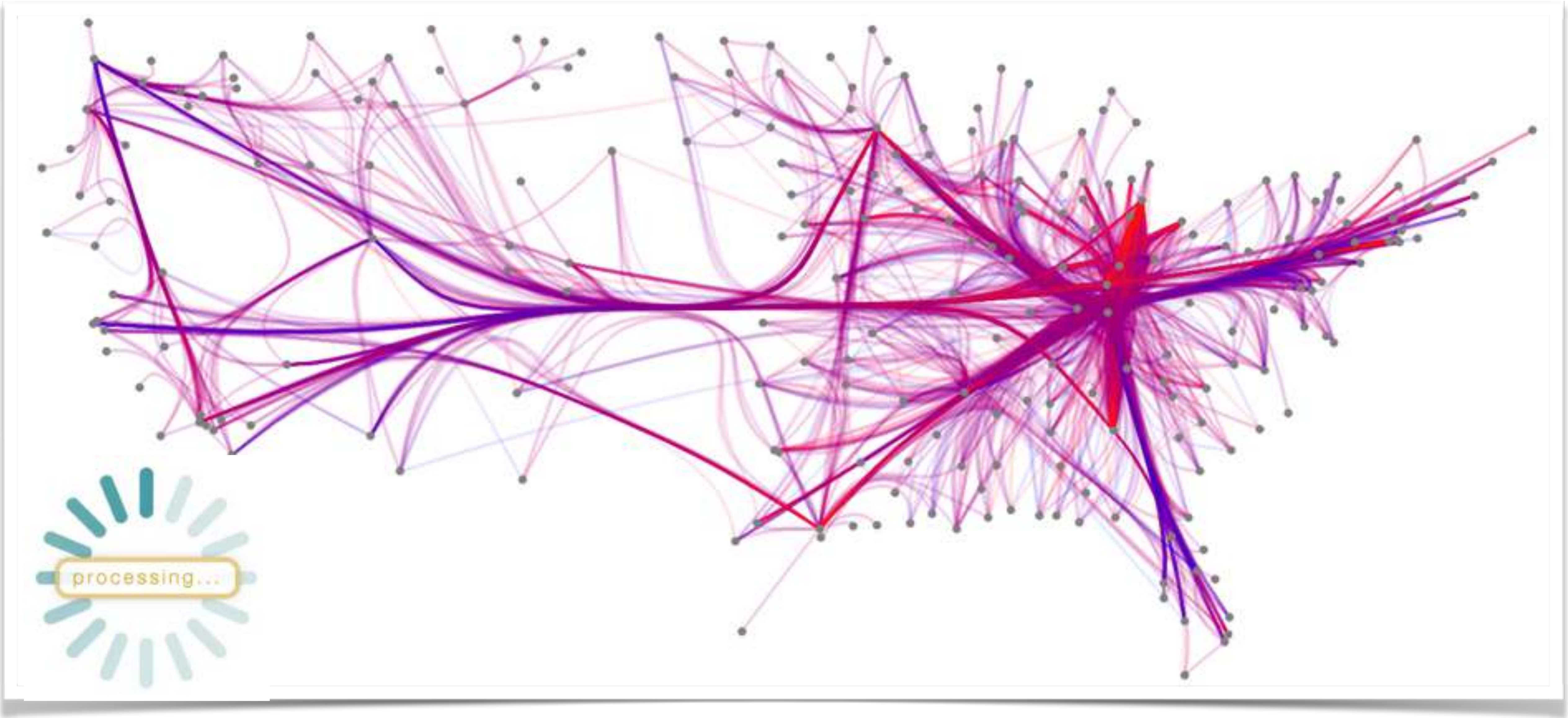
1	0.01	0.41	[illegible]	0.01	0.41
0.01	[illegible]	.4.3	0.01	0.9	0.43
0.41	0.92	[illegible]	0.41	0.92	0.92
0.922	0.01	0.41	1	[illegible]	0.41
0.01	0.9	[illegible]	0.01	1	.4.3
0.41	0.92	0.92	0.41	0.92	1

1	0	0	1	0	0
0	1	0	0	1	0
0	1	1	0	1	1
1	0	0	1	0	0
0	1	0	0	1	0
0	1	1	1	1	1

processing

Slow

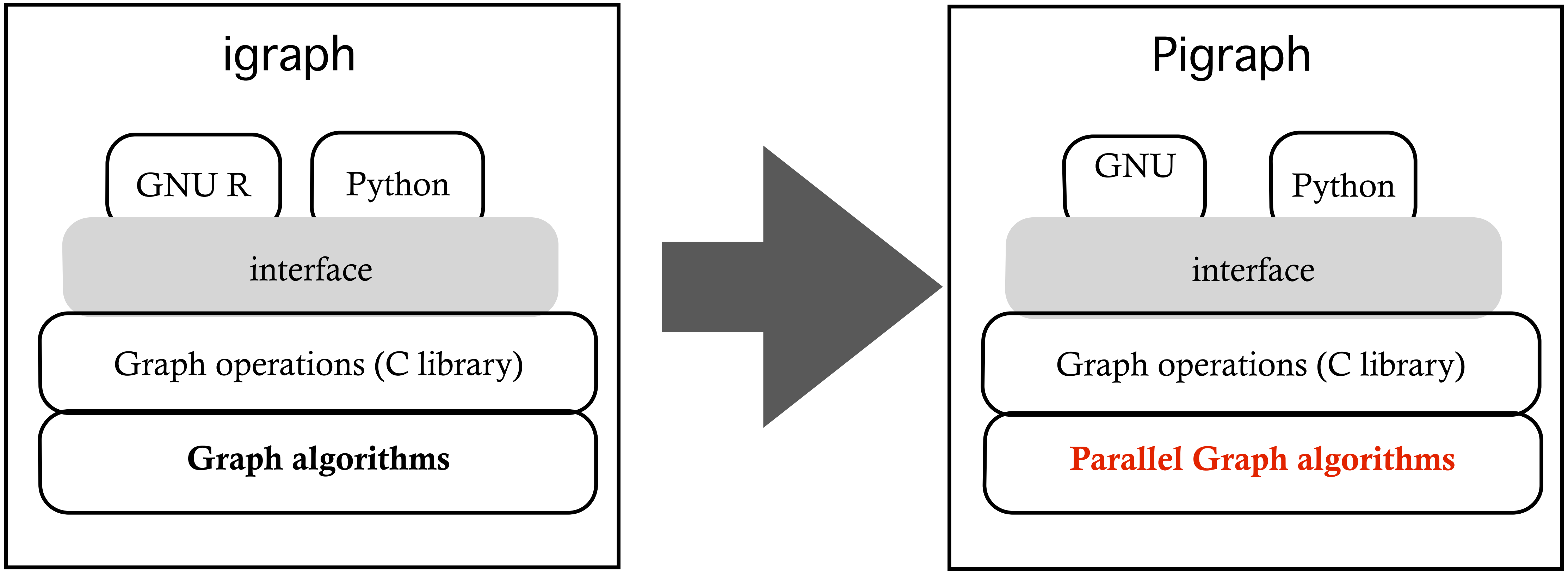
- parallel reading?
- data reduction/compression?
- parallel tools to analyze complex networks?



Parallel tools to analyze complex networks

Pigraph

Pigraph – parallel library for graph analysis



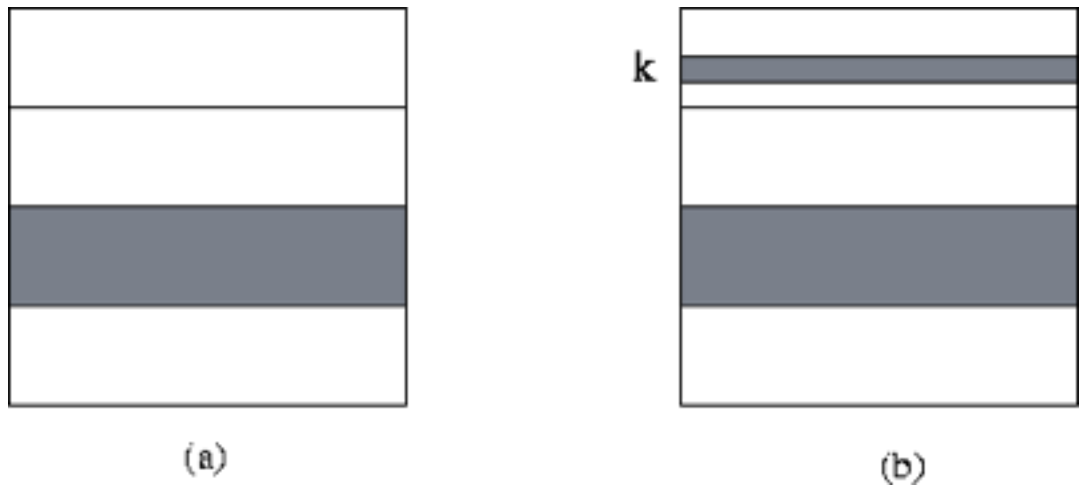
igraph
GNU R
Python
interface
Graph operations (C library)
Graph algorithms
Pigraph
GNU
Python
interface
Graph operations (C library)
Parallel Graph algorithms

- ➡ OpenMP
- ➡ Shared memory platforms

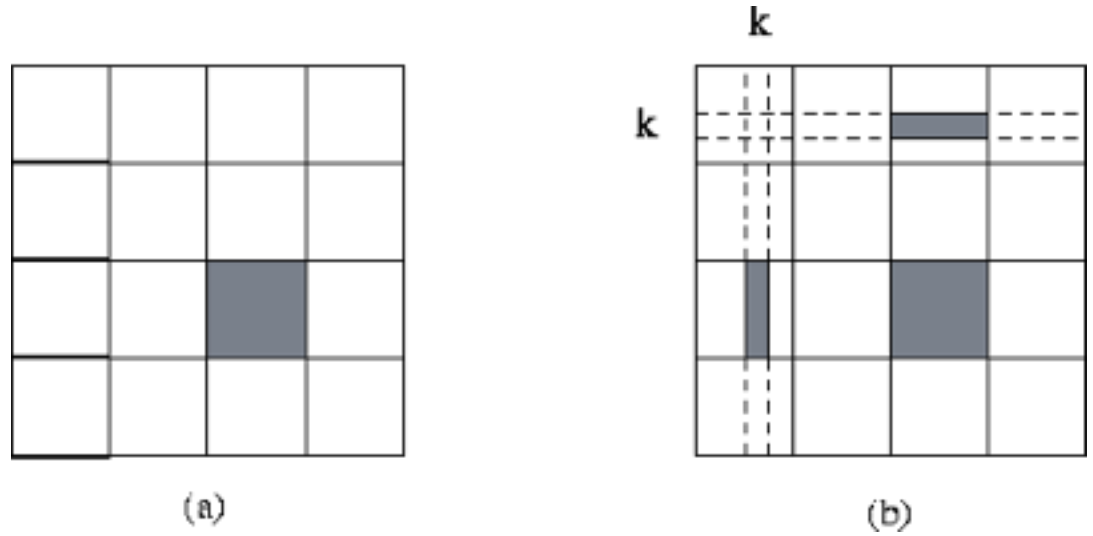
Pigraph – example: "shortest path": Floyd-Warshall algorithm

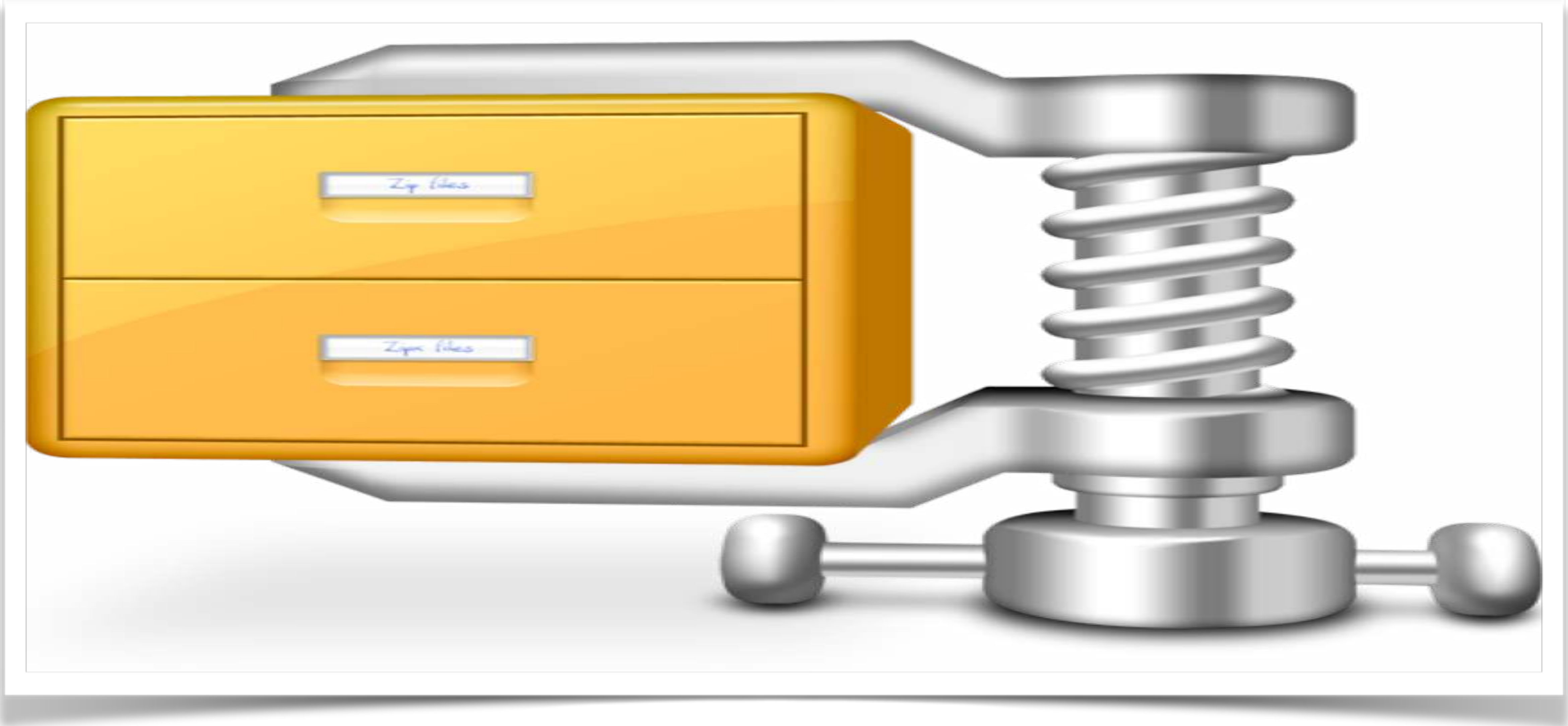
$$D(0) = \begin{bmatrix} 0 & 3 & 8 & \infty & -4 \\ \infty & 0 & \infty & 1 & 7 \\ \infty & 4 & 0 & \infty & \infty \\ 2 & \infty & -5 & 0 & \infty \\ & & & & \end{bmatrix} \longrightarrow D_{(k-1)} = \begin{bmatrix} 0 & 3 & 8 & \infty & -4 \\ \infty & 0 & \infty & 1 & 7 \\ \infty & 4 & 0 & \infty & \infty \\ 2 & 5 & -5 & 0 & -2 \\ \infty & \infty & \infty & 6 & 0 \end{bmatrix}$$

```
For k=1 to n {              Parallel
 For i=1 to n {
     For j=1 to n
        D[i,j] = min(D[i,j],D[i,k]+D[k,j])
 }
}
```



```
For k=1 to n {              Parallel
 For i=1 to n {             Parallel
     For j=1 to n
        D[i,j] = min(D[i,j],D[i,k]+D[k,j])
 }
}
```

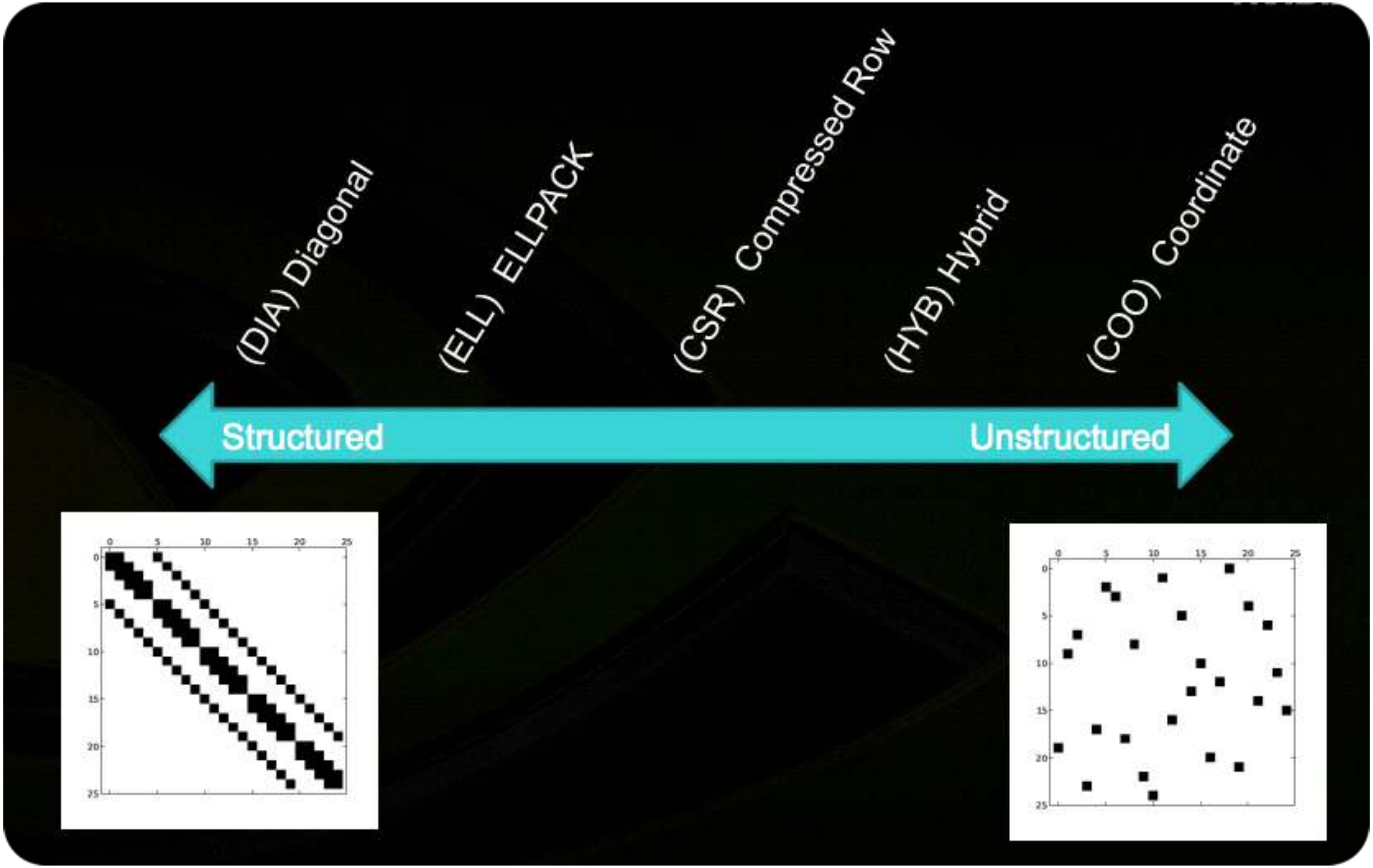




Data reduction / compression

CSR

Compressed sparse matrices



(DIA) Diagonal

(ELL) ELLPACK

(CSR) Compressed Row

(HYB) Hybrid

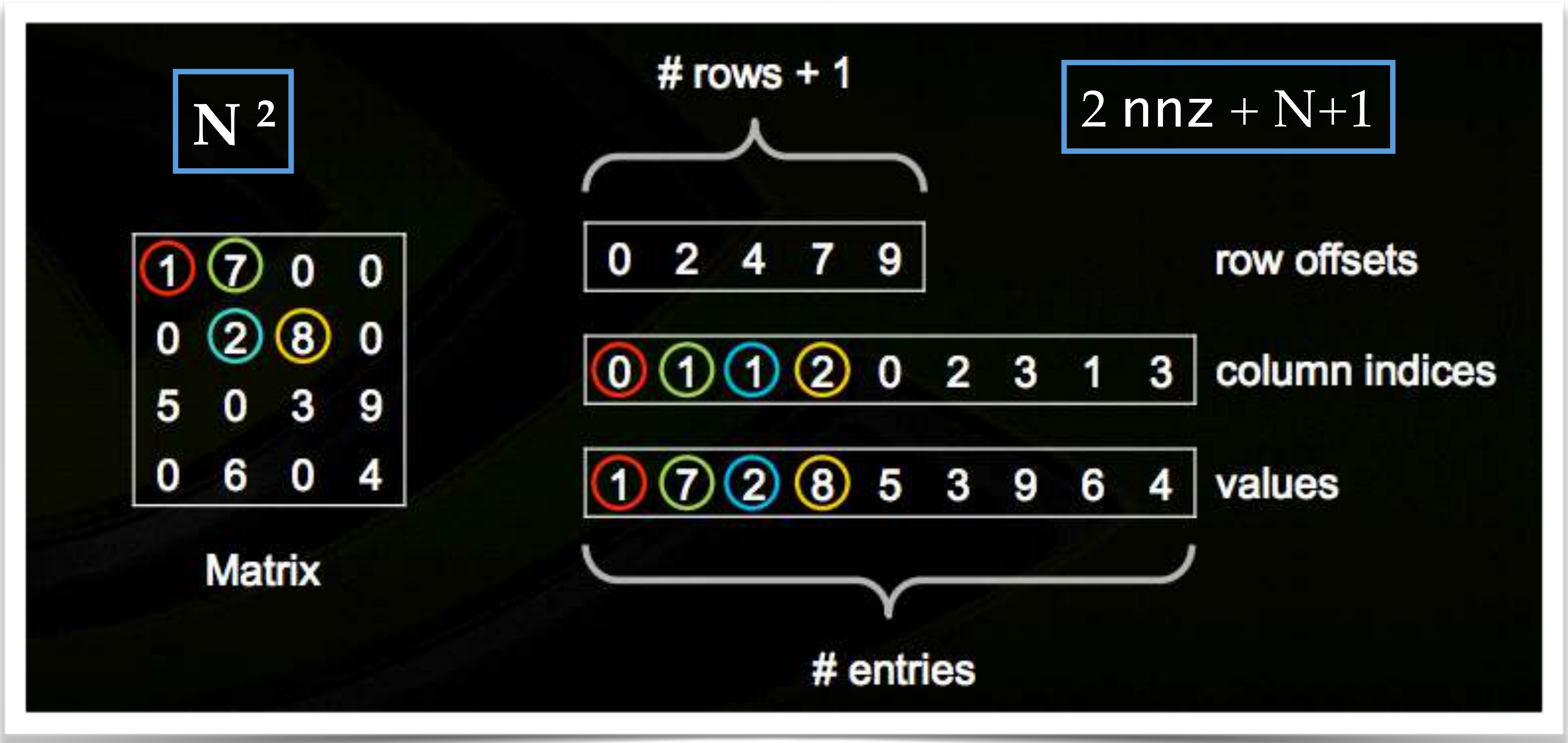
(COO) Coordinate

Structured

Unstructured

Compressed sparse matrices

Compressed Sparse Row (CSR)



N^2

$2\ \mathrm{nnz} + N+1$

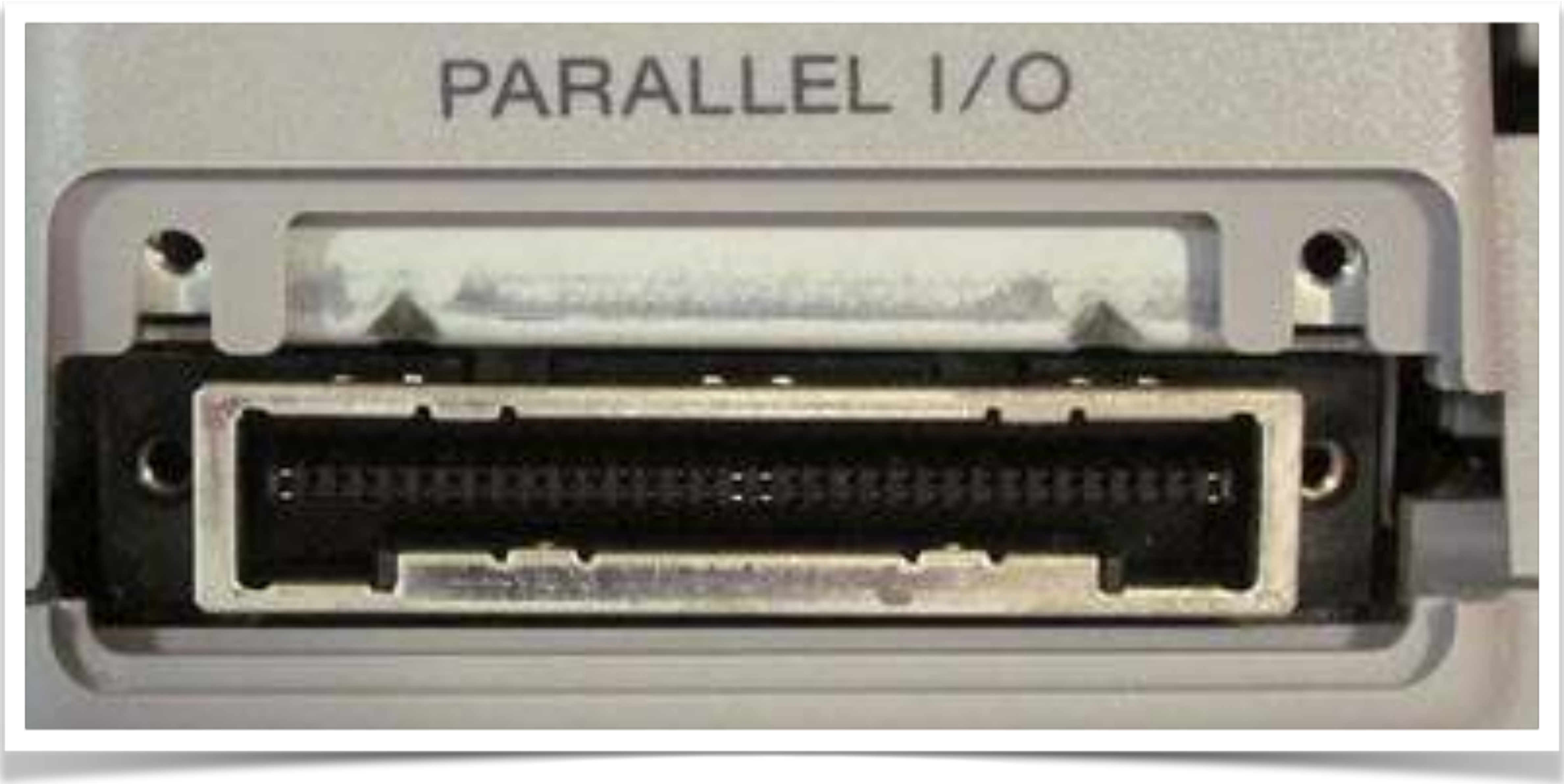
$$\begin{matrix} 1 & 7 & 0 & 0 \\ 0 & 2 & 8 & 0 \\ 5 & 0 & 3 & 9 \\ 0 & 6 & 0 & 4 \end{matrix}$$

Matrix

rows + 1

row offsets	0	2	4	7	9				
column indices	0	1	1	2	0	2	3	1	3
values	1	7	2	8	5	3	9	6	4

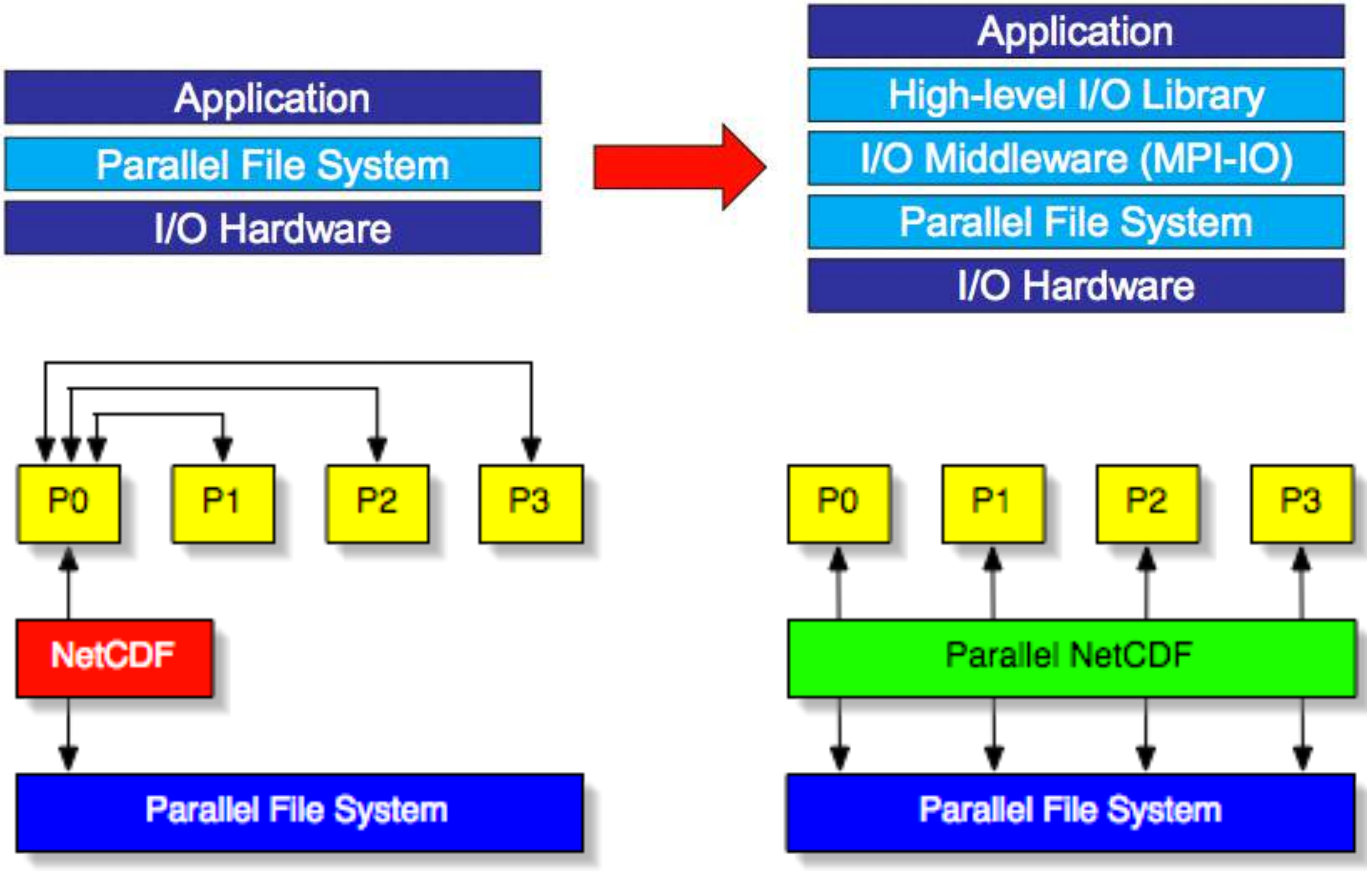
entries



Parallel reading

NetCDF-4 (HDF5, MPI/IO)

Parallel I/O



Application

Parallel File System

I/O Hardware

Application

High-level I/O Library

I/O Middleware (MPI-IO)

Parallel File System

I/O Hardware

P0

P1

P2

P3

NetCDF

Parallel File System

P0

P1

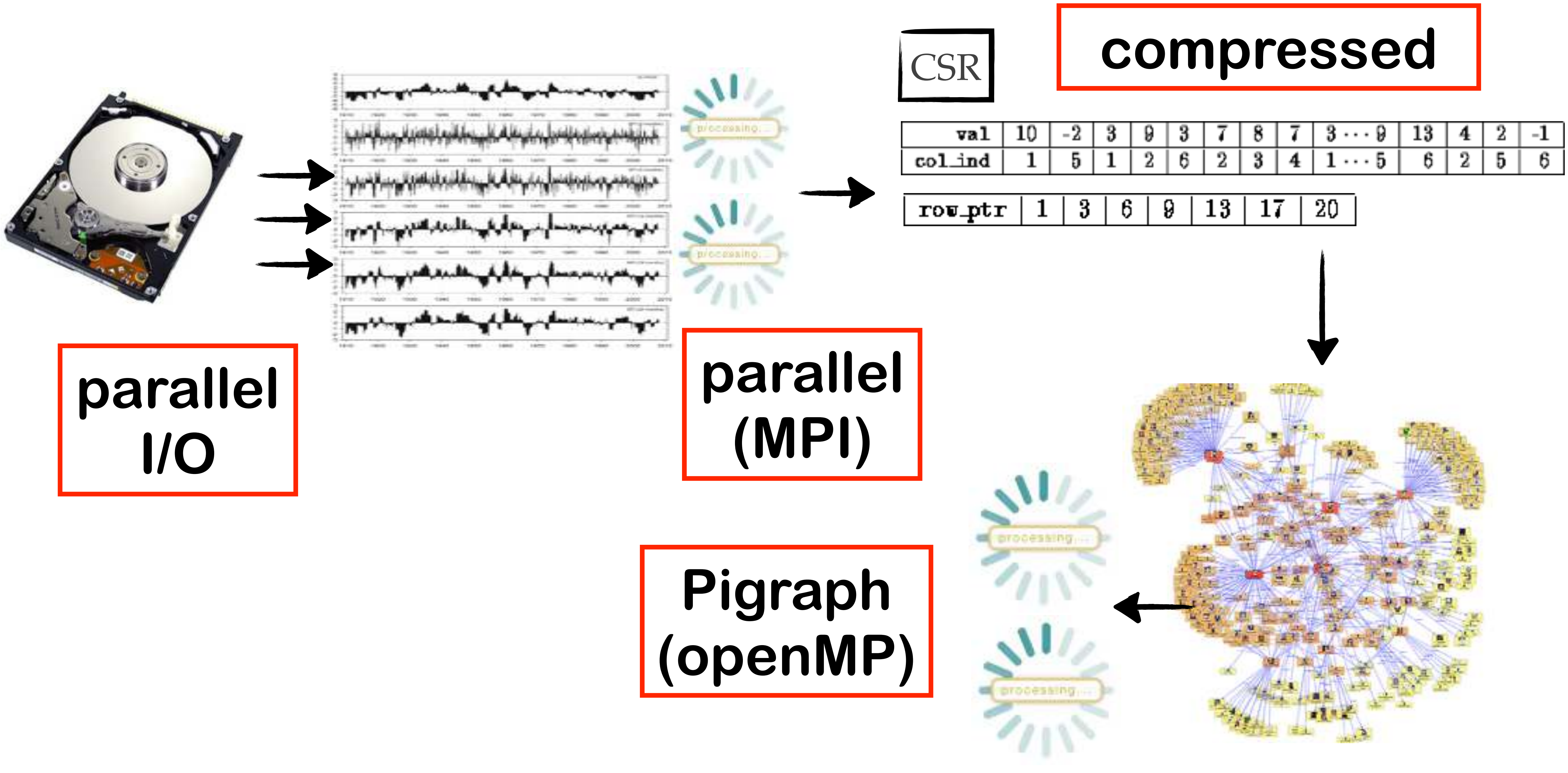
P2

P3

Parallel NetCDF

Parallel File System

Parallel software tools for the construction and analysis of complex networks



parallel I/O

parallel (MPI)

CSR

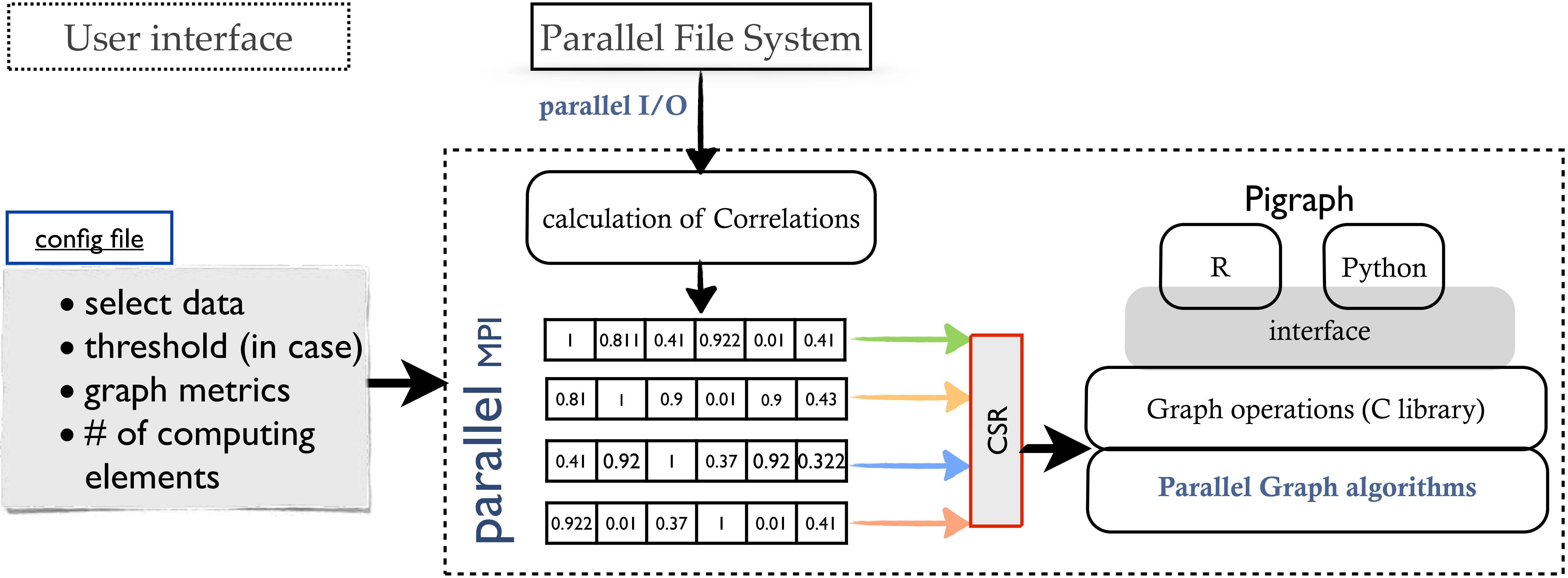
compressed

val	10	-2	3	9	3	7	8	7	3 ··· 9	13	4	2	-1
col_ind	1	5	1	2	6	2	3	4	1 ··· 5	6	2	5	6

row_ptr	1	3	6	9	13	17	20

Pigraph (openMP)

Parallel software tools for the construction and analysis of complex networks



User interface

Parallel File System

parallel I/O

config file

- select data
- threshold (in case)
- graph metrics
- # of computing elements

parallel MPI

calculation of Correlations

1	0.811	0.41	0.922	0.01	0.41
0.81	1	0.9	0.01	0.9	0.43
0.41	0.92	1	0.37	0.92	0.322
0.922	0.01	0.37	1	0.01	0.41

CSR

Pigraph

R

Python

interface

Graph operations (C library)

Parallel Graph algorithms

Thanks!