Knowledge Discovery Toolkit Status Report

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KDT Spring Mind Meld
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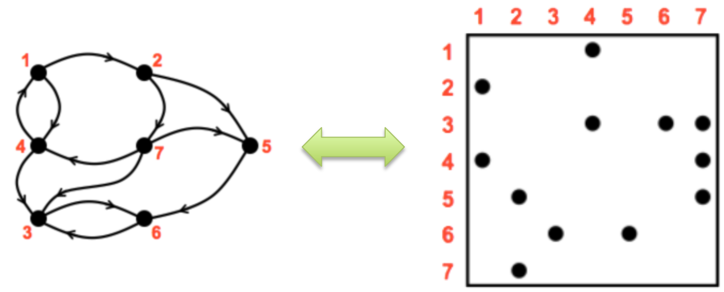
Support: Intel, Microsoft, DOE Office of Science, NSF

K**nowledge**
D**iscovery**
T**oolbox**

http://kdt.sourceforge.net/



A general graph library with operations based on linear algebraic primitives

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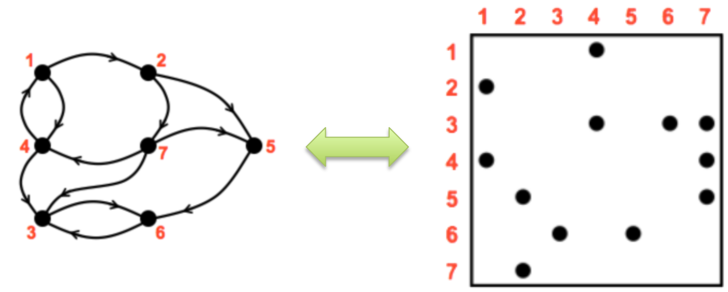

A general graph library with operations based on linear algebraic primitives

- Aimed at domain experts who know their problem well but don't know how to program a supercomputer
- Easy-to-use Python interface
- Runs on a laptop as well as a cluster with 10,000 processors

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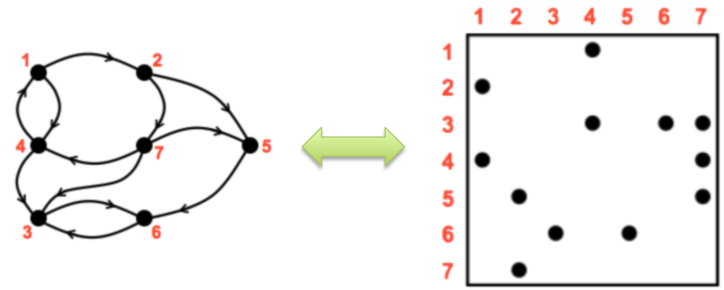

A general graph library with operations based on linear algebraic primitives

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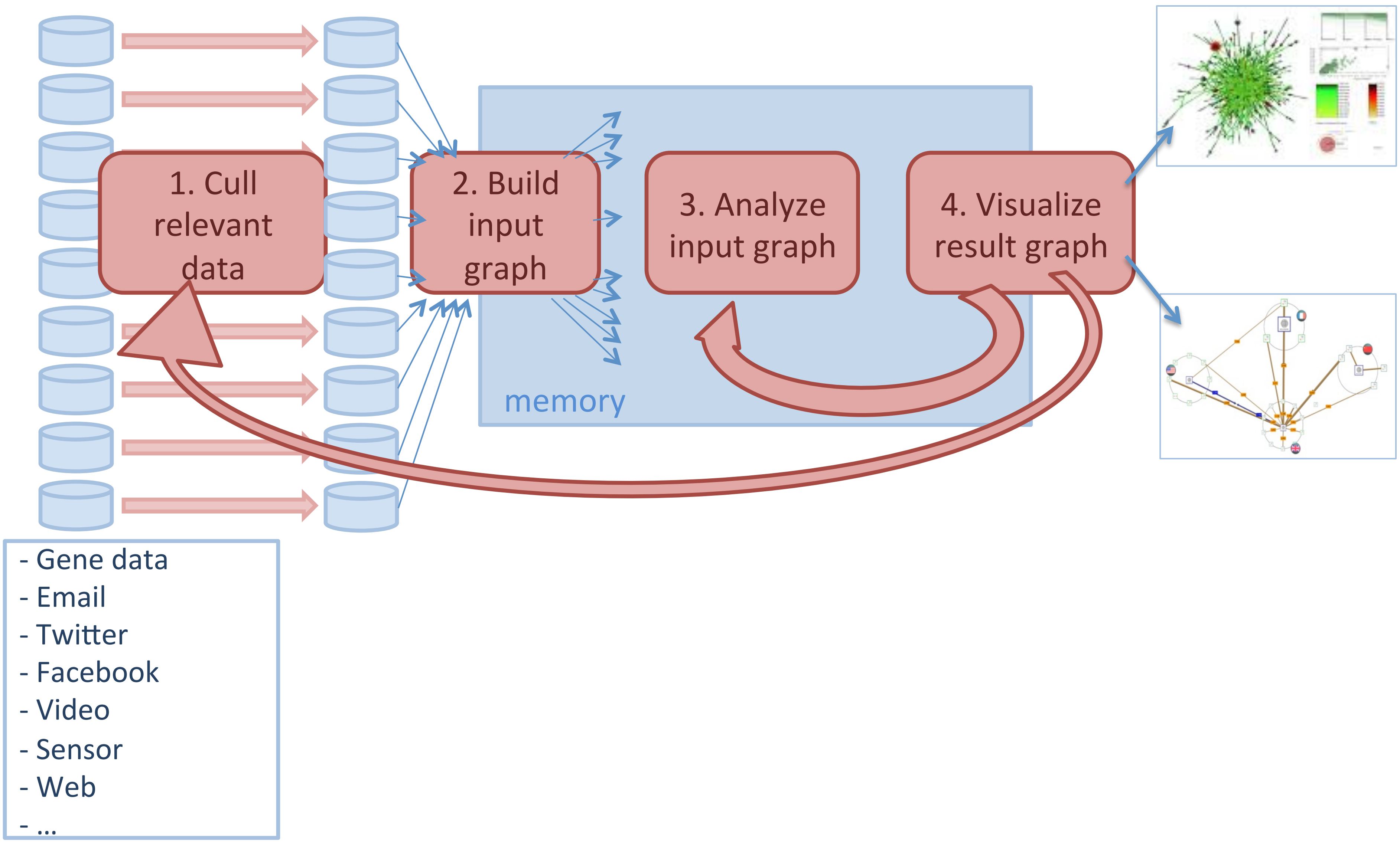
- A collaboration among UCSB, UCB, and Lawrence Berkeley Lab
- Open source software, released under New BSD license
- v0.1 released March 2011; v0.2 expected March 2012

Knowledge Discovery Workflow



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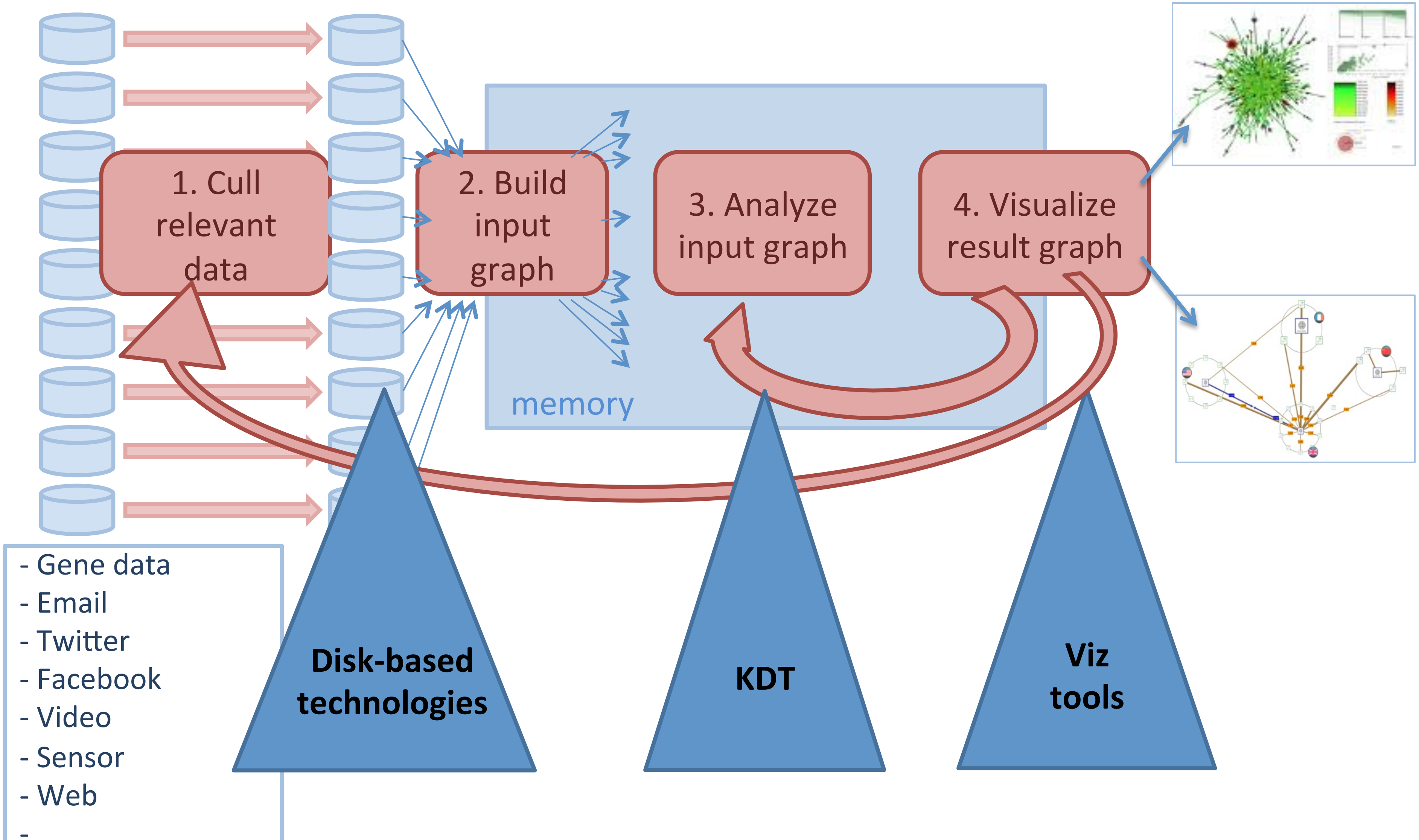

Domain Expert vs. Graph Expert

- (Semantic) directed graphs
  - constructors, I/O
  - basic graph metrics (*e.g.*, `degree()`)
  - vectors
- Clustering / components
- Centrality / authority: betweenness centrality, PageRank

- Hypergraphs and sparse matrices
- Graph primitives (*e.g.*, `bfsTree()`)
- SpMV / SpGEMM on semirings

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```
# bigG contains the input graph
comp = bigG.connComp()
giantComp = comp.hist().argmax()
G = bigG.subgraph(comp==giantComp)

clus = G.cluster('Markov')

clusNedge = G.nedge(clus)

smallG = G.contract(clus)

# visualize
```

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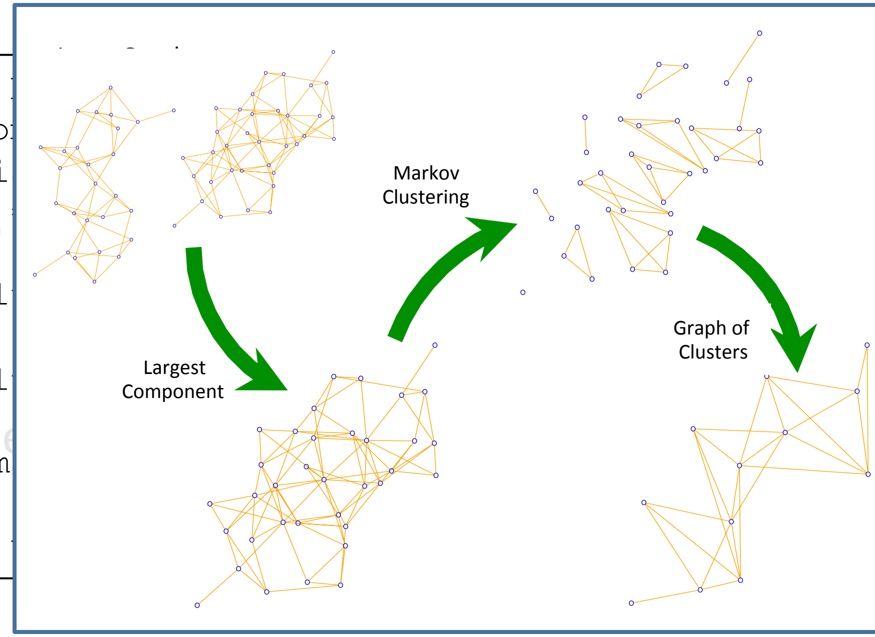
```
#
co
gi
G

cl

cl

sm

#
```



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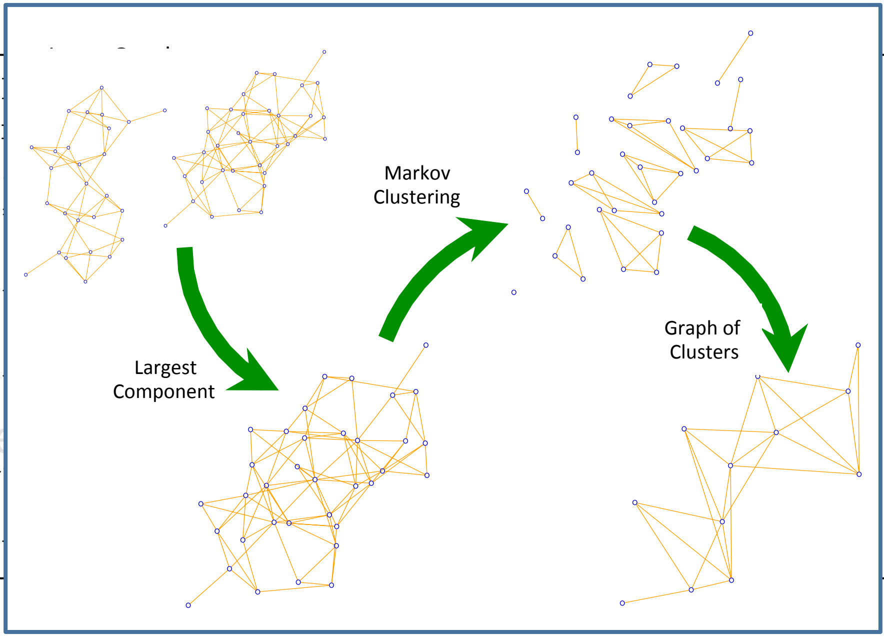

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```
            [...]
L = G.toSpParMat()
d = L.sum(kdt.SpParMat.Column)
L = -L
L.setDiag(d)
M = kdt.SpParMat.eye(G.nvert()) - mu*L
pos = kdt.ParVec.rand(G.nvert())
for i in range(nsteps):
    pos = M.SpMV(pos)
```

A few KDT applications

Markov Clustering

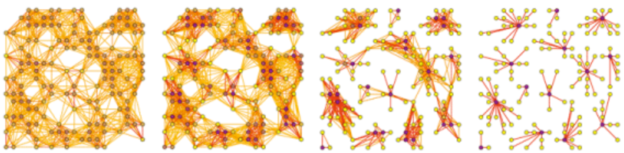


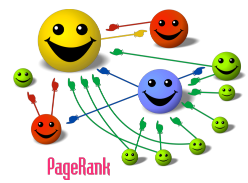
image courtesy Stijn van Dongen

Markov Clustering (MCL) finds clusters by postulating that a random walk that visits a dense cluster will probably visit many of its vertices before leaving.

We use a Markov chain for the random walk. This process is reinforced by adding an inflation step that uses the Hadamard product and rescaling.

PageRank

PageRank says a vertex is important if other important vertices link to it.

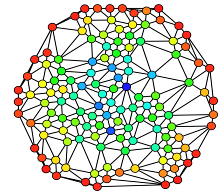


courtesy Felipe Micaroni Lalli

Each vertex (webpage) votes by splitting its PageRank score evenly among its out edges (links). This broadcast (an SpMV) is followed by a normalization step (ColWise). Repeat until convergence.

PageRank is the stationary distribution of a Markov Chain that simulates a "random surfer".

Betweenness Centrality

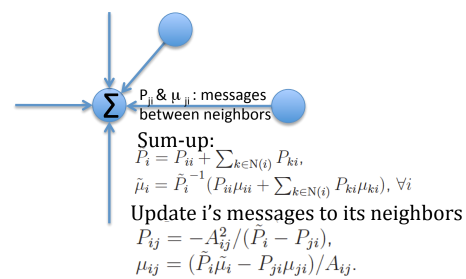


$$C_B(v) = \sum_{\substack{s \neq v \neq t \in V \\ s \neq t}} \frac{\sigma_{st}(v)}{\sigma_{st}}$$

image courtesy Claudio Rocchini

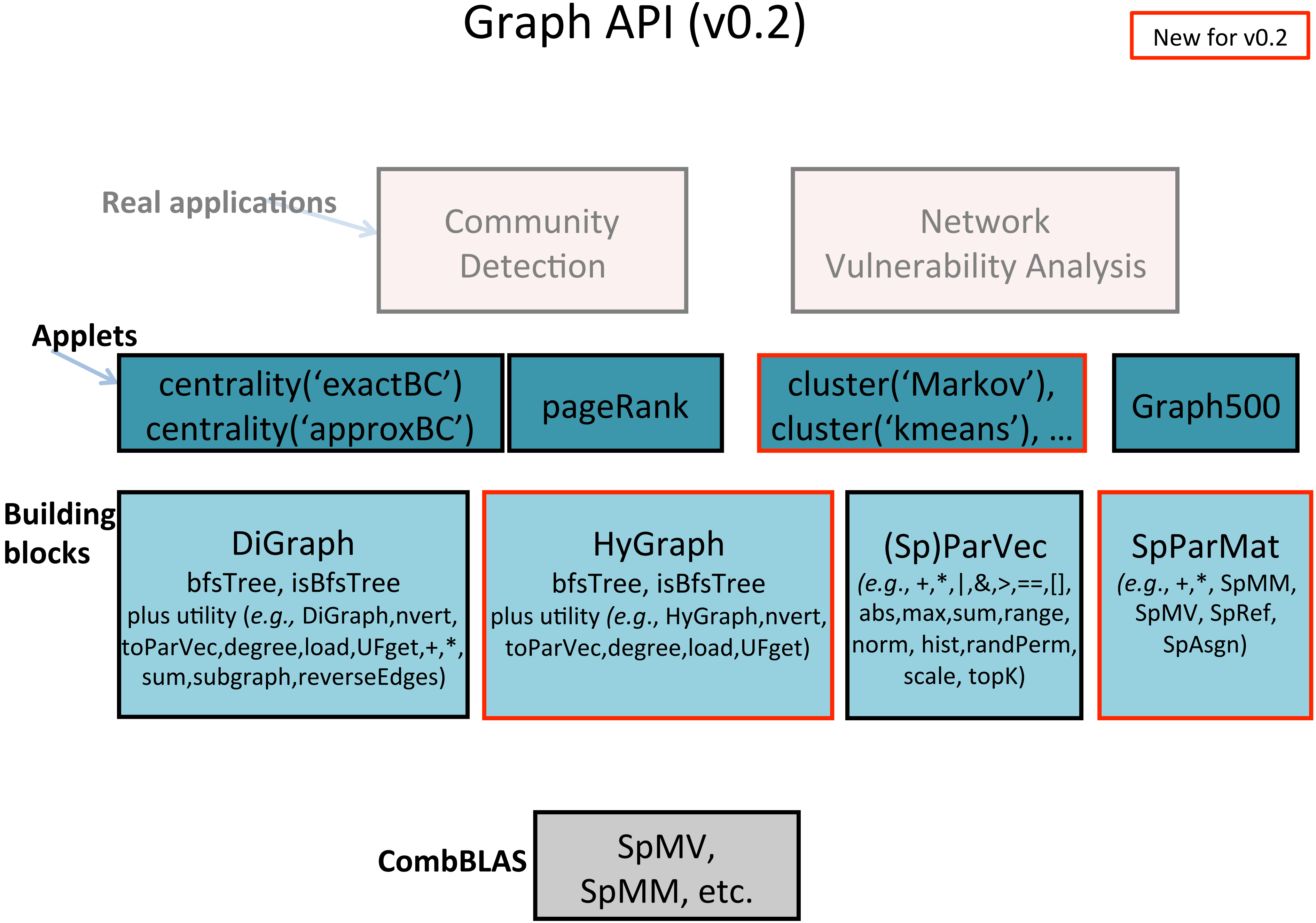
Betweenness Centrality says that a vertex is important if it appears on many shortest paths between other vertices. An exact computation requires a BFS for every vertex. A good approximation can be achieved by sampling starting vertices.

Belief Propagation

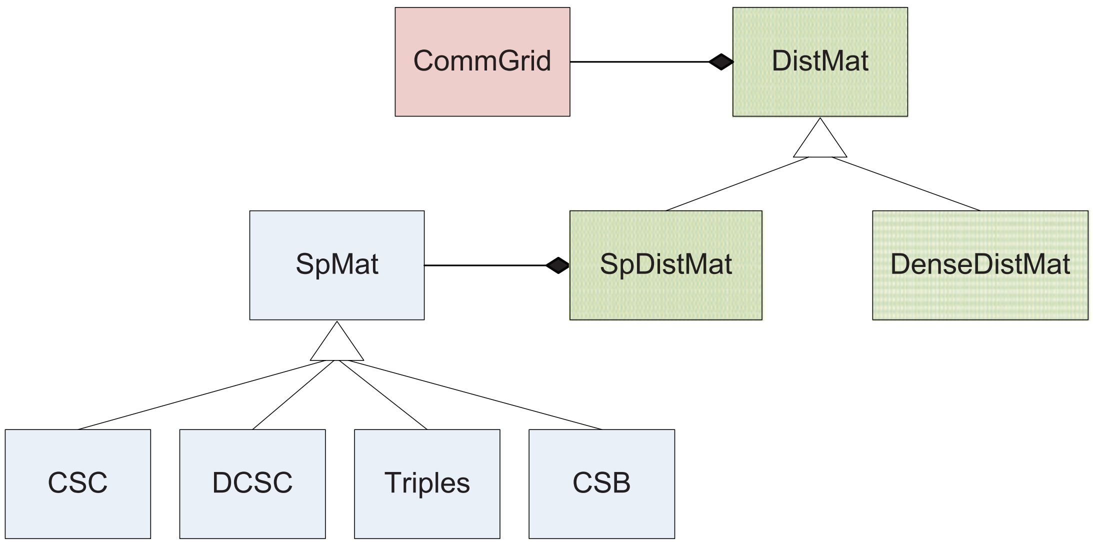


Gaussian belief propagation (GaBP) is an iterative algorithm for solving the linear system of equations Ax = b, where A is symmetric positive definite.
GaBP assumes each variable follows a normal distribution. It iteratively calculates the precision P and mean value μ of each variable; the converged mean-value vector approximates the actual solution.

Graph API (v0.2)



Combinatorial BLAS: A matrix-based graph library



Architecture of matrix classes

- Also sparse & dense vectors, distributed and local
- Matrix operations over user-defined (and some built-in) semirings
- Highly templated C++
- Reference implementation in MPI

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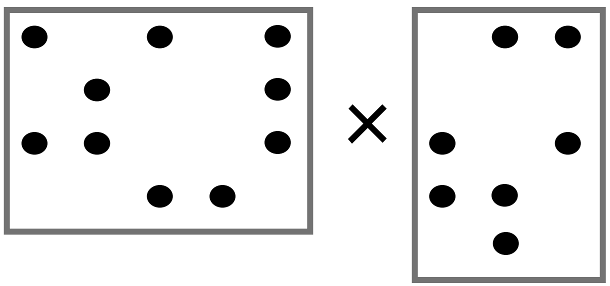
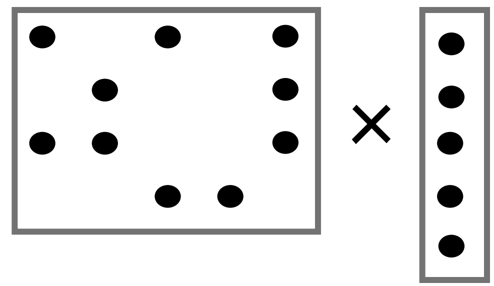
Sparse array-based primitives

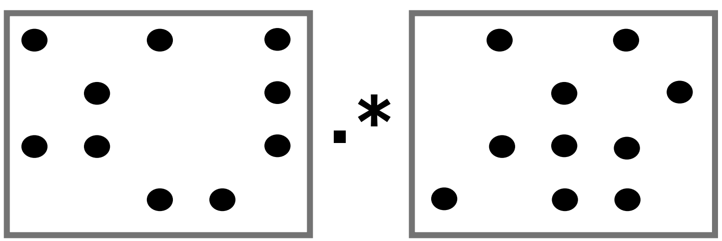
Sparse matrix-matrix multiplication (SpGEMM)



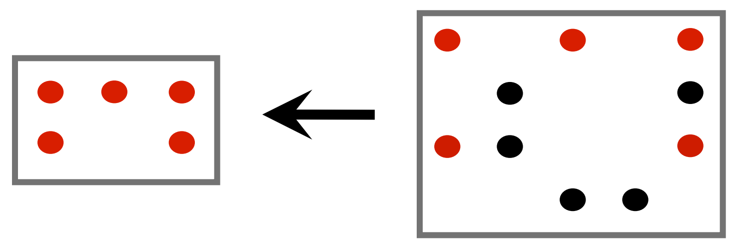
Sparse matrix-dense vector multiplication



Element-wise operations



Sparse matrix indexing

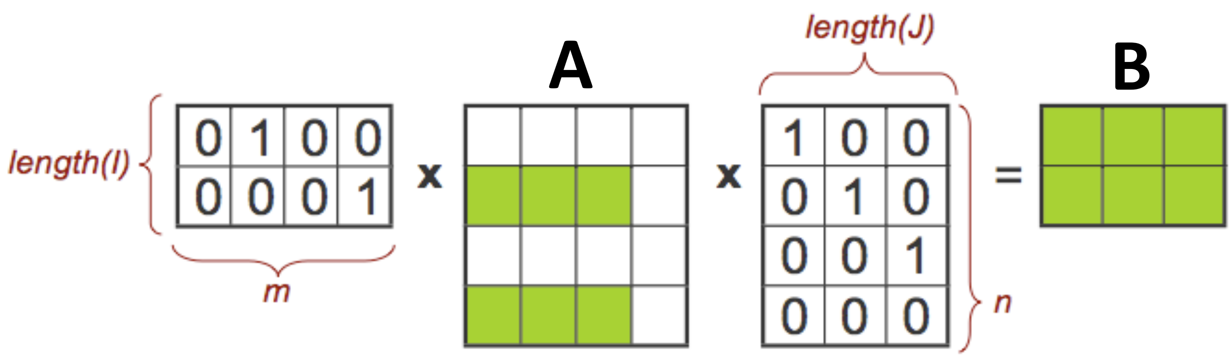


Matrices on various semirings: (x, +) , (and, or) , (+, min) , …

Indexing sparse arrays in parallel
(coarsen graphs, extract subgraphs, etc.)

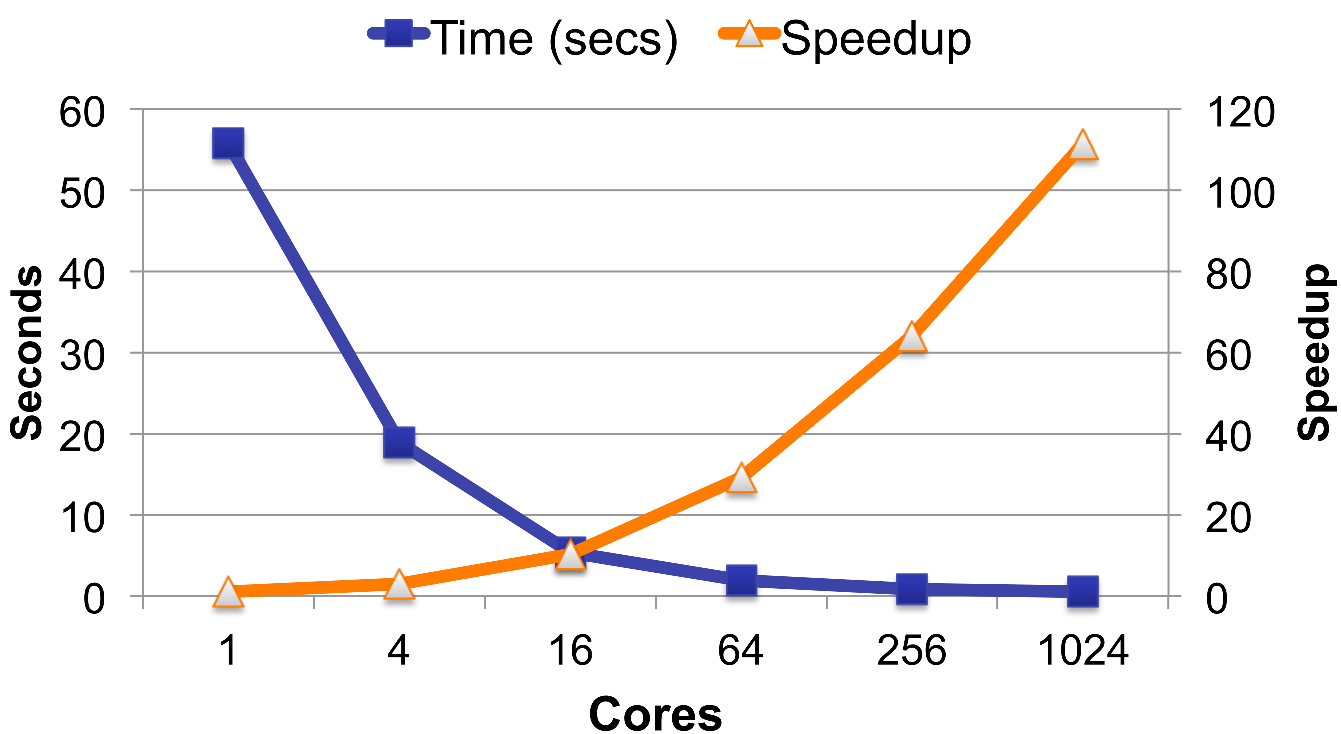
SpRef: B = A(I,J)
SpAsgn: B(I,J) = A
SpExpAdd: B(I,J) += A

A,B: sparse matrices
I,J: vectors of indices



SpRef using mixed-mode sparse matrix-matrix multiplication (**SpGEMM**). Ex: B = A([2,4], [1,2,3])

Strong scaling of SpRef



random symmetric permutation ⇔ relabeling graph vertices

- RMAT Scale 22; edge factor=8; a=.6, b=c=d=.4/3
- Franklin/NERSC, each node is a quad-core AMD Budapest

KDT v0.2: Attributed Semantic Graphs and Filters

Example:

- Vertex types: Person, Phone, Camera
- Edge types: PhoneCall, TextMessage, CoLocation
- Edge attributes: StartTime, EndTime

- Calculate centrality just for PhoneCalls and TextMessages between times sTime and eTime

```
def vfilter(self, vTypes):
    return self.type in vTypes

def efilter(self, eTypes, sTime, eTime):
    return ((self.type in eTypes) and
            (self.sTime > sTime) and
            (self.eTime < eTime))


wantedVTypes = (People)
wantedETypes = (PhoneCall, TextMessage)
start = dt.now() - dt.timedelta(hours=1)
end = dt.now()
bc = G.centrality('approxBC',filter=
        ((vfilter, wantedVTypes),
         (efilter, wantedETypes,
          start, end)))
```

Implementing filters: Options

- Prefilter to extract the relevant subgraph
  - Simple, but too much time / memory for many use cases
- Write filters in Python, call back from CombBLAS
  - Simple & flexible, but hurts performance
- Write filters as semiring ops in C++, wrap in Python
  - Good performance, but hard to write new filters
- Work in progress: Write filters in Python subset, compile with SEJITS (selective embedded just-in-time specialization)

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KDT Team (2011-12)

- David Alber, Microsoft
- Victor Amelkin, UCSB
- Aydin Buluc, LBNL
- Varad Deshmukh, UCSB
- Kevin Deweese, UCSB
- John Gilbert, UCSB
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- Steve Reinhardt, Cray
- Lijie Ren, UCSB
- Veronika Strnadova, UCSB
- Yun Teng, UCSB
- Drew Waranis, UCSB

- Support: Intel, Microsoft, DOE Office of Science, NSF

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