Enabling Rapid Development and Execution of Advanced Graph-Analysis Algorithms on Very Large Graphs

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Knowledge Discovery Toolbox (KDT) embodies two key innovations:

Technically

- Technically, non-graph-expert subject-matter experts analyze terascale graphs with multiple advanced algorithms with leading performance

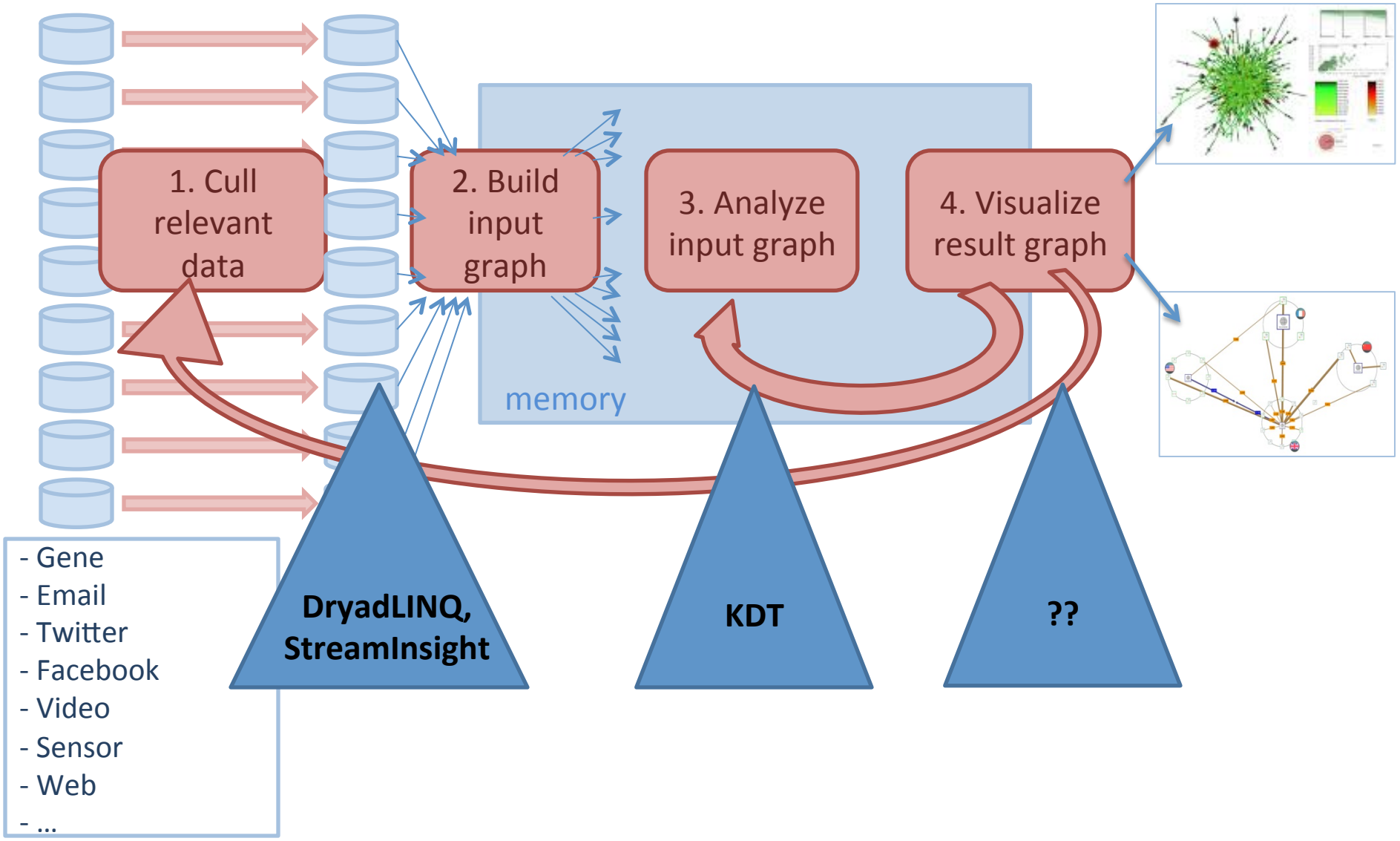
Architecturally

- Architecturally, graph algorithm users, graph algorithm developers, and graph infrastructure developers each use complementary interfaces to advance the field

Agenda

- APIs for different audiences
- Semantic and hyper-graphs
- Implementation / performance

KNOWLEDGE DISCOVERY WORKFLOW



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- APIs for different audiences
- Semantic and hyper-graphs
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KDT APIs enable disparate groups' work to reinforce each other

Technically

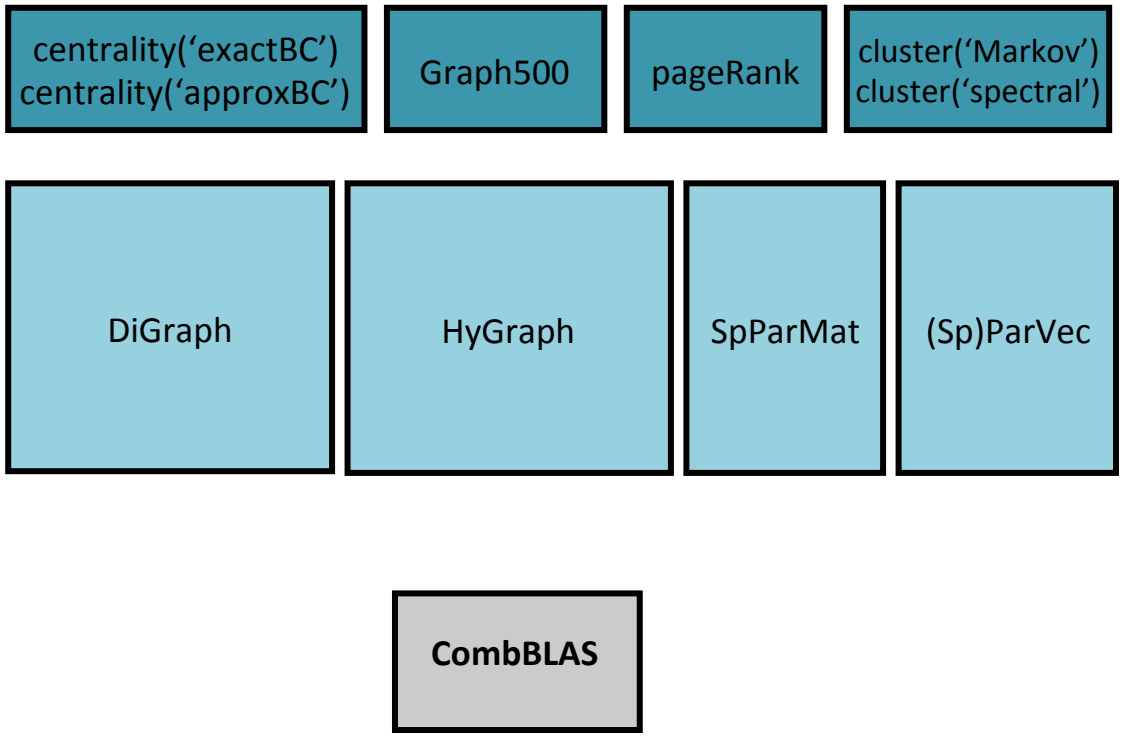
Architecturally

- Fosters earlier use and learning about how algorithms work at scale

Graph-algorithm users
develop applications based on a set of complex graph algorithm implemented by experts

Graph-algorithm developers
develop algorithms for a growing set of users through an evolving set of interfaces, based on powerful infrastructure

Graph-infrastructure developers
develop new implementations of the KDT interfaces for different hardware or software platforms



KDT APIs enable disparate groups' work to reinforce each other

Technically

Architecturally

Graph-algorithm users

Graph-algorithm developers

Graph-infrastructure developers

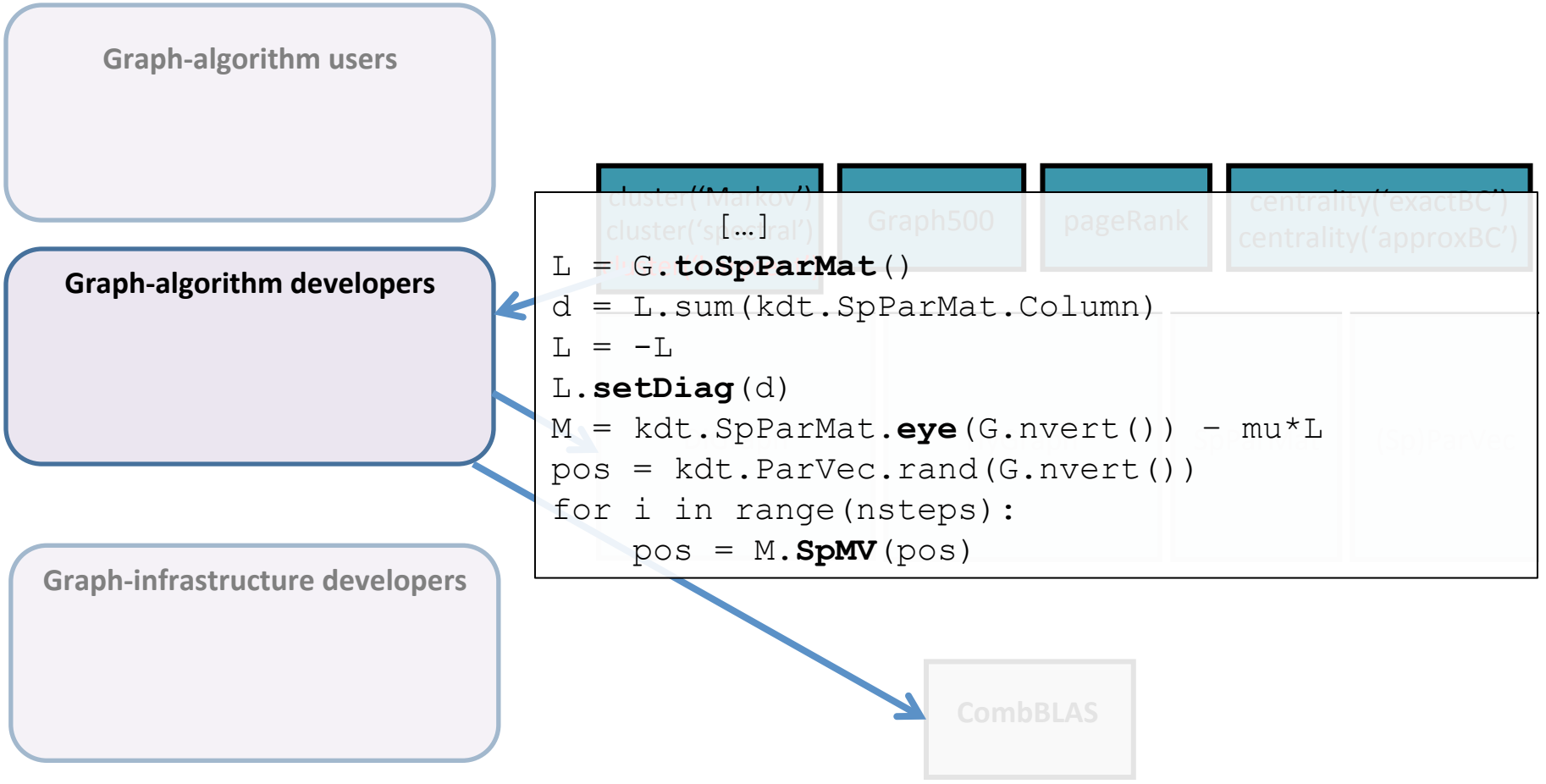
```
# Graph500.py
deg3verts = (G.degree() > 2).findInds()
deg3verts.randPerm()
starts = deg3verts[kdt.ParVec.range(nstarts)]
G.toBool()
[origI, ign, ign2] = G.toParVec()
for start in starts:
    parents = G.bfsTree(start, sym=True)
    nedges = len((parents[origI] != -1).find())
    if not k2Validate(G, start, parents):
        verifyResult = "FAILED"
```

CombBLAS

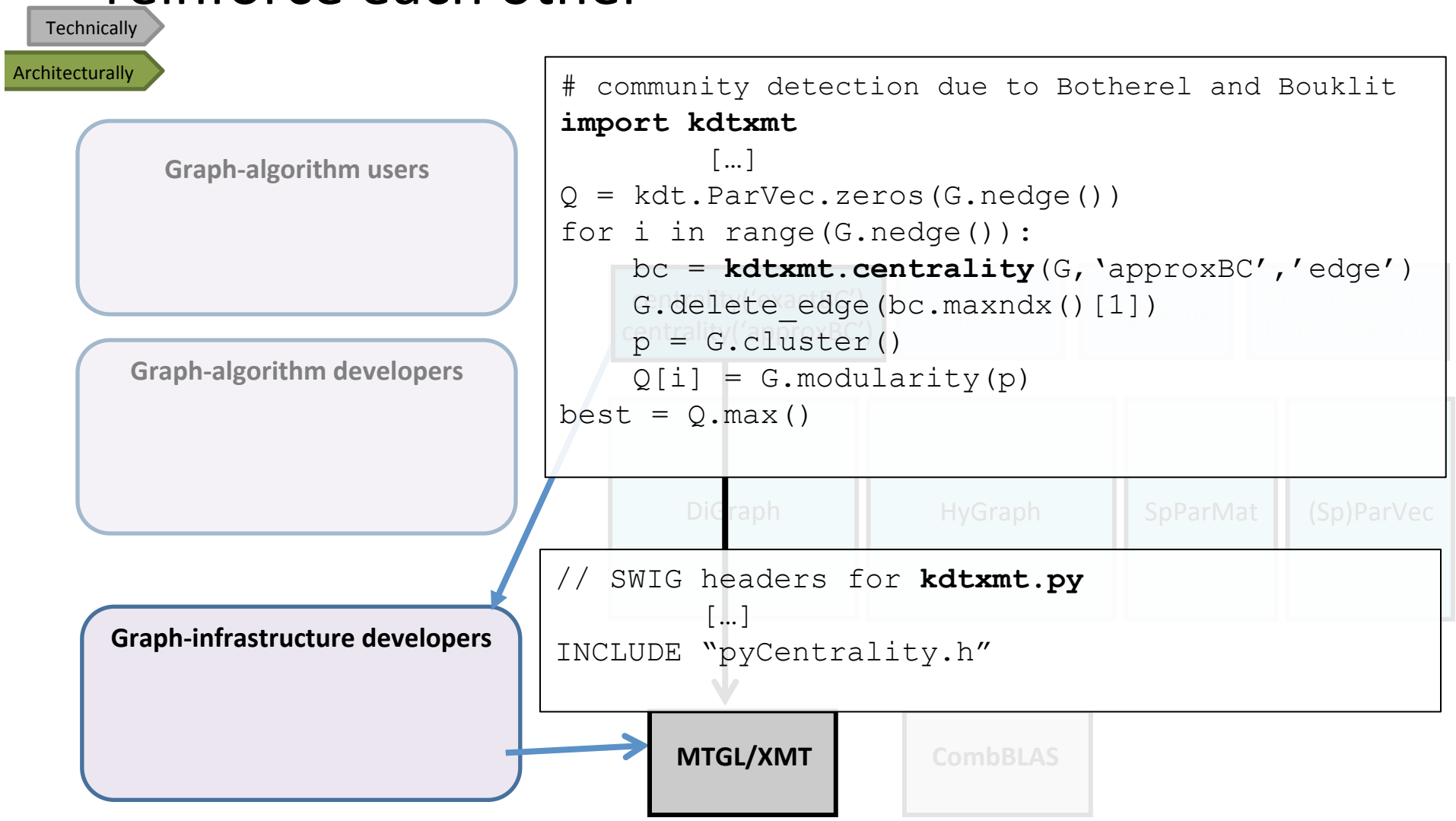
KDT APIs enable disparate groups' work to reinforce each other

Technically

Architecturally



KDT APIs enable disparate groups' work to reinforce each other



KDT's Graph API (v0.1)

Technically

Architecturally

- Targeted at non-graph-expert domain experts
- Exposed via Python

Real applications

Community Detection

Network Vulnerability Analysis

Applets

centrality('exactBC')
centrality('approxBC')

Graph500

pageRank

Building blocks

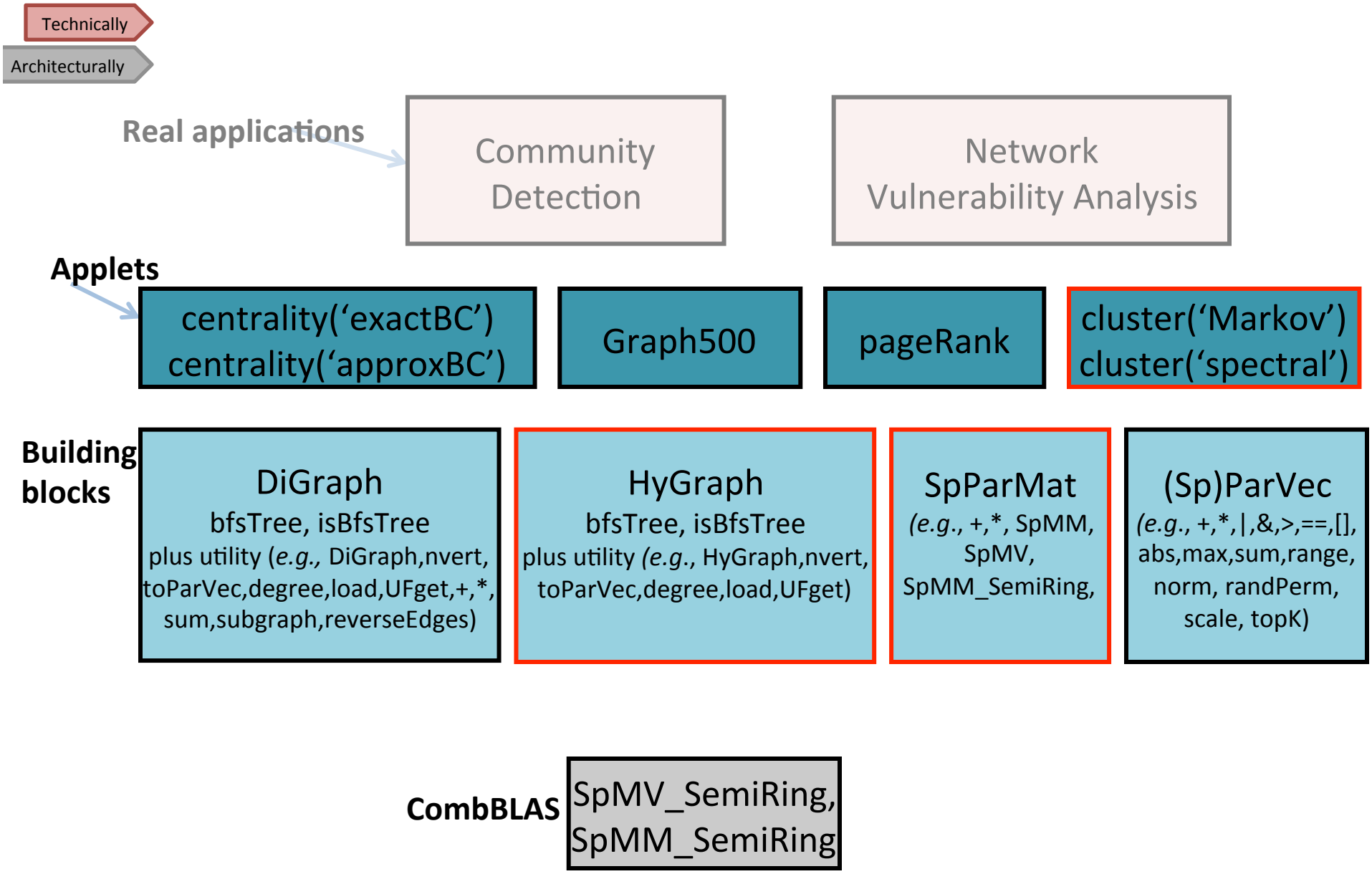
DiGraph
bfsTree, isBfsTree
plus utility (*e.g.,* DiGraph,nvert, toParVec,degree,load,UFget,+,*, sum,subgraph,reverseEdges)

(Sp)ParVec
(*e.g.*, +,*,|,&,>,==,[], abs,max,sum,range, norm, randPerm, scale, topK)

CombBLAS

SpMV_SemiRing,
SpMM_SemiRing

KDT's Graph API (v0.2)



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Semantic-graph API: Multiple Criteria

Technically

Architecturally

Level of abstraction

Customiz-ability

Performance

CombBLAS

- Atypical abstractions
+ Sustainably scalable performance

PBGL

- Abstractions low-level for domain experts
+ Scalable performance

KDT v0.2 goal

Semantic Graph Use Case

- Vertex types: Person, SmartPhone, Camera
- Edge types: PhoneCall, TextMessage, PhysicalPresence
- Edge StartTime, EndTime:

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

Approach 1: Known Good Performance

Technically

Architecturally

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

def efilter(self, wantedETypes, sTime, eTime):
    return kdt.and(kdt.in(wantedETypes, self.type),
              kdt.and(kdt.gt(sTime, self.sTime),
                      kdt.lt(eTime, self.eTime)))

wantedVTypes = (People)
wantedETypes = (PhoneCall, TextMessage)
bc = Gtmp.centrality('approxBC',filter=(vfilter,efilter))
```

Approach 2: Highly Flexible, Currently Bad Performance

Technically

Architecturally

```
def vfilter(self, wantedVTypes):
    # any Python constructs permitted
    return self.type in wantedVTypes

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

wantedVTypes = (People)
wantedETypes = (PhoneCall, TextMessage)
bc = G.centrality('approxBC',filter=(vfilter,efilter))
```

Approach 3: Likely Good Performance, but Potentially Memory-Expensive

Technically

Architecturally

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

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

wantedVTypes = (People)
wantedETypes = (PhoneCall, TextMessage)
Gtmp = G.subgraph(filter=(vfilter,efilter))
bc = Gtmp.centrality('approxBC')
```

Hypergraph Support

- The underlying sparse matrix is interpreted as an incidence matrix; vertices are in columns, edges in rows
- (Subset of) same methods implemented
- Graph500 Kernel 2 looks identical except validation
- Performance not yet measured for big cases, but expected to take twice as long as same DiGraph method
  - Two SpMVs in the core loop instead of one
  - TEPS rating the same

bfsTree

Technically

Architecturally

DiGraph

```
def bfsTree(self, root, sym=False):

if not sym:
    self._T()
parents = pcb.pyDenseParVec(self.nvert(), -1)
fringe = pcb.pySpParVec(self.nvert())
parents[root] = root
fringe[root] = root
while fringe.getnee() > 0:
    fringe.setNumToInd()
    self._spm.SpMV_SelMax_inplace(fringe)

    pcb.EWiseMult_inplacefirst(fringe, parents, True, -1)
    parents[fringe] = 0
    parents += fringe
if not sym:
    self._T()
return ParVec.toParVec(parents)
```

HyGraph

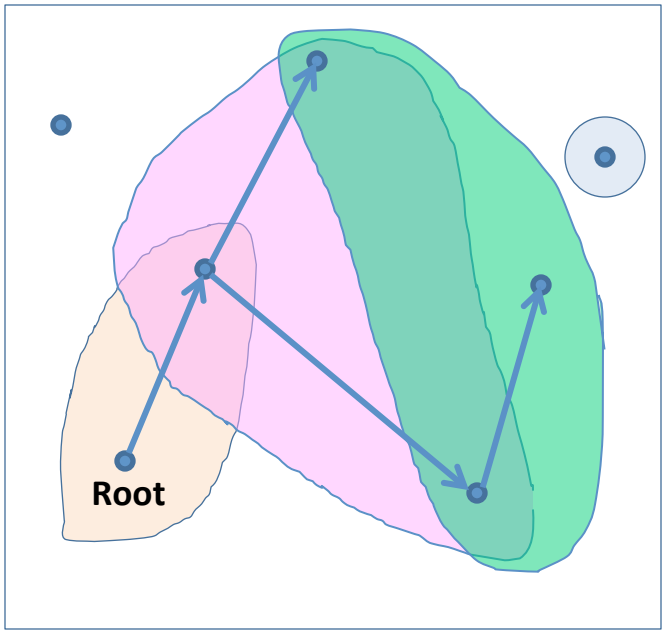
```
def bfsTree(self, root):


parents = pcb.pyDenseParVec(self.nvert(), -1)
fringeV = pcb.pySpParVec(self.nvert())
parents[root] = root
fringeV[root] = root
while fringeV.getnee() > 0:
    fringeV.setNumToInd()
    fringeE = self._spm.SpMV_SelMax(fringeV)
    fringeV = self._spmT.SpMV_SelMax(fringeE)
    pcb.EWiseMult_inplacefirst(fringeV, parents, True, -1)
    parents[fringeV] = 0
    parents += fringeV


return ParVec.toParVec(parents)
```

Questions about Hypergraph Support

Technically

Architecturally

- We have defined a BFS tree of a hypergraph as a set of simple edges, each contained in a hyperedge (which permits cycles of hyperedges). Is this the most useful definition?
- Are hypergraphs in the KDT style useful? What use cases should we target? What methods should we provide?



Agenda

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Key DiGraph Methods in KDT v0.1/v0.2

Technically

Architecturally

```
def pageRank(self, epsilon=0.1, dampingFactor=0.85):
def centrality(self, alg, **kwargs):
    'exactBC',normalize=True
    'approxBC', sample=0.05, normalize=True
def cluster(self, alg, **kwargs):
    'Markov'
    'spectral'
def bfsTree(self, root, sym=False):
def isBfsTree(self, root, parents, sym=False):
def neighbors(self, source, nhop=1, sym=False):
def pathsHop(self, source, sym=False):

def degree(self, dir=gr.Out):
def genGraph500Edges(self, scale):
def load(fname):
def UFget(fname):
def max(self, dir):
def reverseEdges(self):
def scale(self, other, dir=gr.Out):
def sum(self, dir):
def DiGraph(sourceV, destV, weight, nvert):
def toParVec(self):
def toBool(self):
def normalizeEdgeWeights(self):
```

```
class Graph: #base class only

class DiGraph:

class ParVec:

class SpParVec:

class SpParMat:


def sendFeedback():
    # may want to disable this
```

Key HyGraph Methods in KDT v0.2

Technically

Architecturally

```
def pageRank(self, epsilon=0.1, dampingFactor=0.85):
def centrality(self, alg, **kwargs):
    'exactBC',normalize=True
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def cluster(self, alg, **kwargs):
def bfsTree(self, root, sym=False):
def isBfsTree(self, root, parents):
def neighbors(self, source, nhop=1):
def pathsHop(self, source):

def degree(self, dir=gr.Out):
def genGraph500Edges(self, scale):
def load(fname):
def UFget(fname):
def max(self, dir):
def invertEdgesVertices(self):
def scale(self, other, dir=gr.Out):
def sum(self, dir):
def HyGraph(edgeNumV, incidentVertexV, weightV, nvert):
def toParVec(self):
def toBool(self):
def toDiGraph(self):
def normalizeEdgeWeights(self):
```
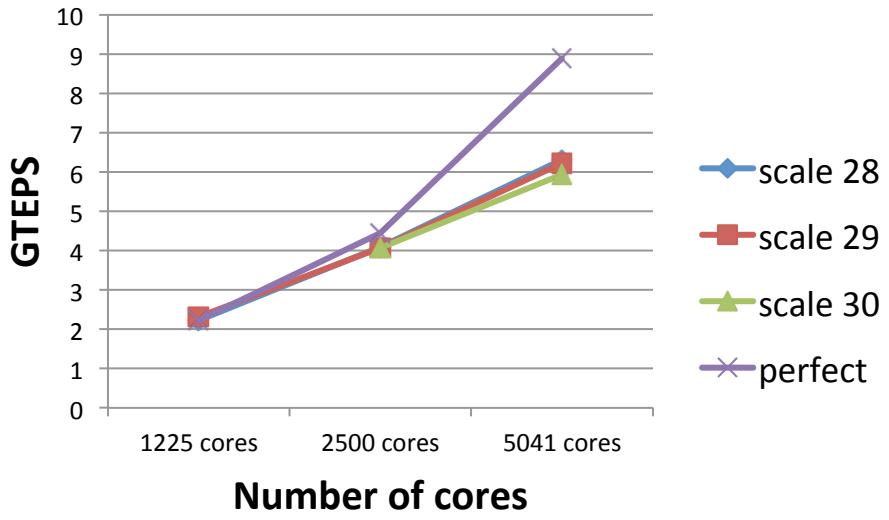

Graph500 Performance [Aydin Buluc]

Technically

Architecturally

- Excellent scaling up to 2500 cores, good to 5K cores
  - LBL/NERSC's Hopper Cray XE6
- Scale 29 ("mini") has 8B directed edges
- Performance measured from Python



- On-node thread parallelism starts to show benefit at 10K cores and above

KDT development and licensing

- KDT is a collaboration among UCSB (John Gilbert *et al*), LBL (Aydin Buluc), and Microsoft Technical Computing
- The resulting software is released under the New BSD license
- v0.1 was released on March 17
  - Tested on Linux x86 and Cray XT configurations
- V0.2 release targeted for early June
- The project homepage is kdt.sourceforge.net
  - Downloads, User Guide, FAQ and bug reporting

Planned KDT v0.2 Content

- Windows HPC Server version
- Semantic graphs
- Hypergraphs
- Clustering - Markov and spectral

- Out-of-core (Dryad-based) version (likely v0.3)
- Cray XMT version
  - Discussing with Cray et al.
- Version based on other graph infrastructures
  - *E.g.,* Parallel Boost Graph Library, SNAP, MultiThreaded Graph Library

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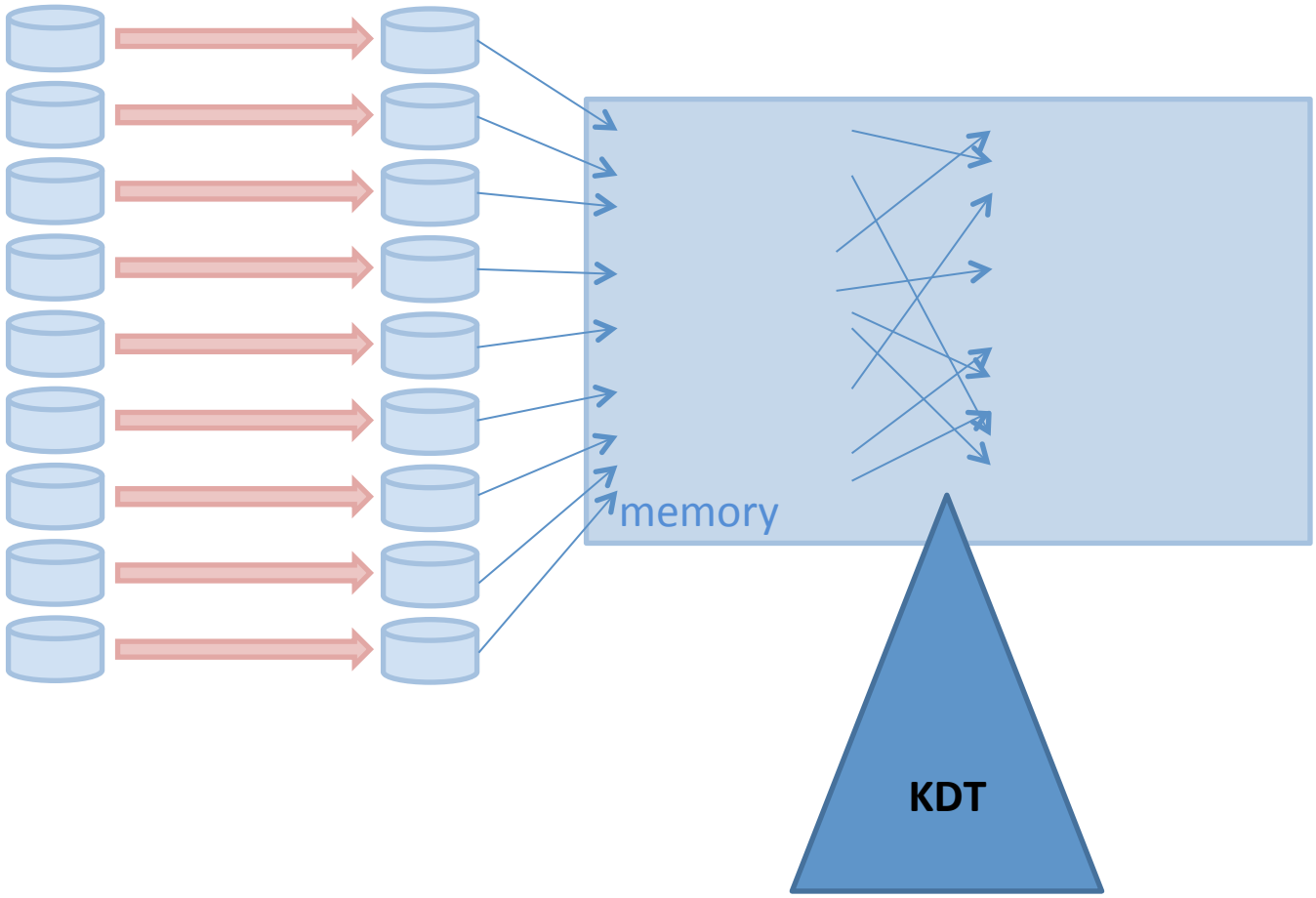
Backup

Graphs-on-Disk Use Case

Technically

Architecturally

Does graph analysis make sense on data that won't all fit in memory?

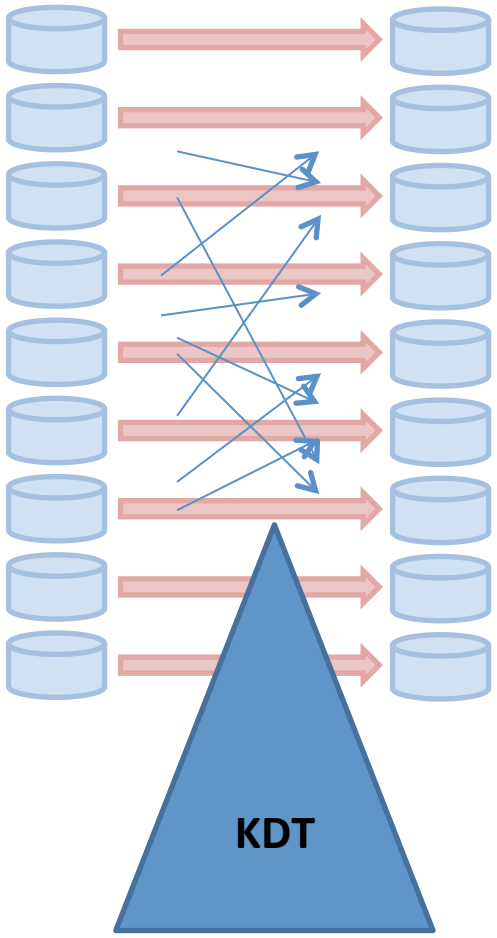


Graphs-on-Disk Use Case

Technically

Architecturally

Does graph analysis make sense on data that won't all fit in memory?



- The sparse-matrix-linear-algebra approach structures communication, so raw pointer-chasing performance not so important
- People are building sparse-matrix packages on top of MapReduce/Hadoop
- We will shortly map the KDT APIs onto a sparse-matrix package based on Dryad*
- Interface perhaps

```
import kdtooc
    […]
G = kdtooc.load('mydata')
G.bfsTree(…)
```

*http://research.microsoft.com/en-us/projects/Dryad/

Questions about KDT-on-disk Support

Technically

Architecturally

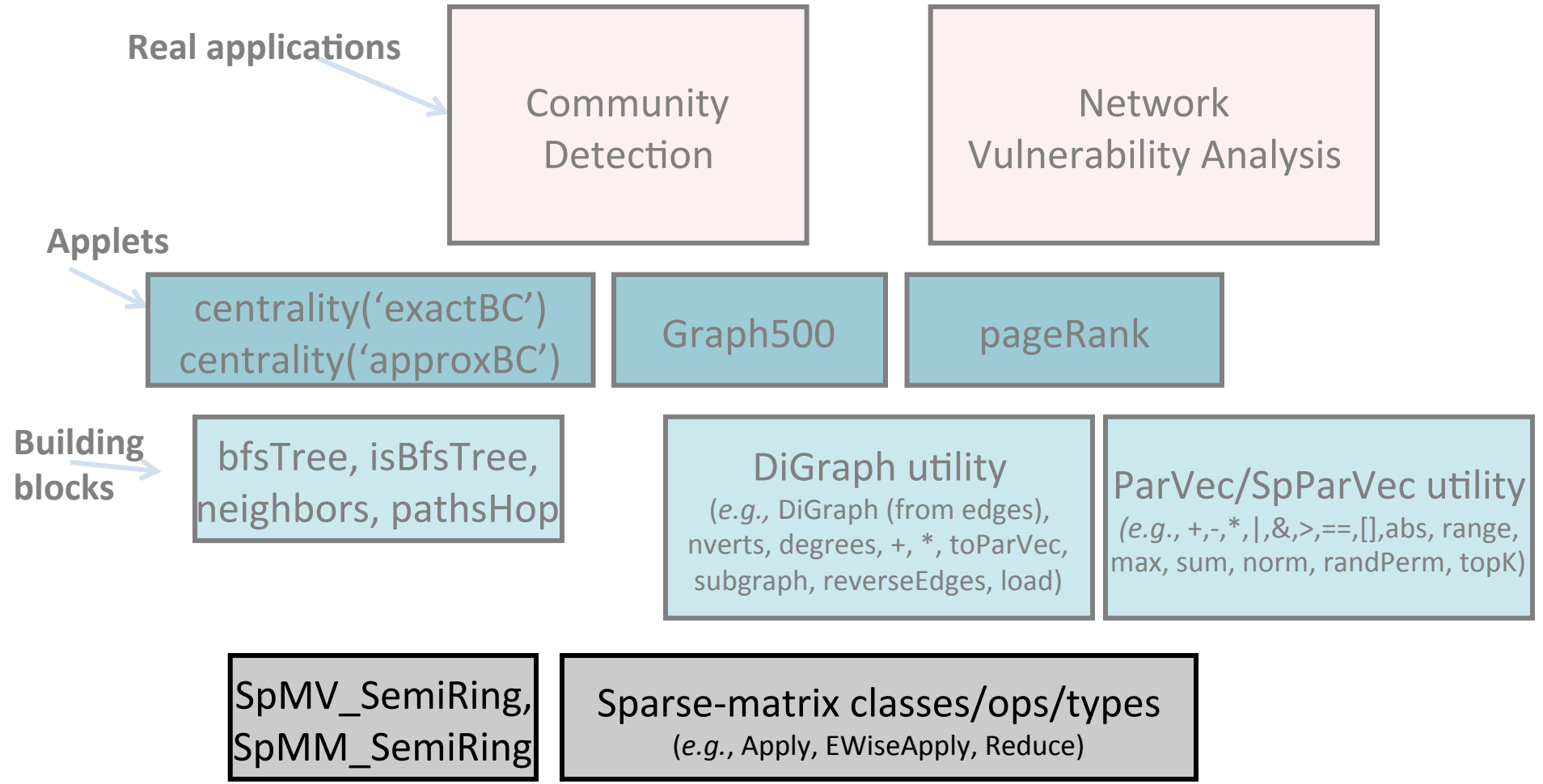
- Assuming that in-memory processing is much faster than on-disk (10X?), what type of graph ops would be practical for on-disk data? Just simple ops? Would something as compute-intensive as BC ever make sense out-of-core?
- Is semantic graph's filtering capability essential for on-disk processing?

KDT Implementation on Combinatorial BLAS

- Combinatorial BLAS
  - Built for combinatorial (sparse-matrix) problems
    - Not limited to simple directed graphs
  - Powers the functionality and performance of KDT
  - Scales well to 2K-4K cores

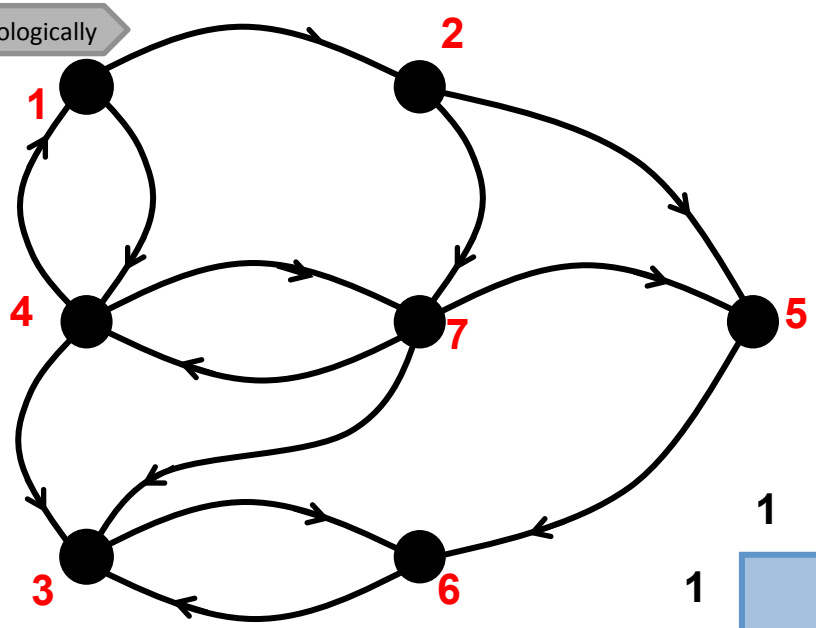
Technically

Ecologically

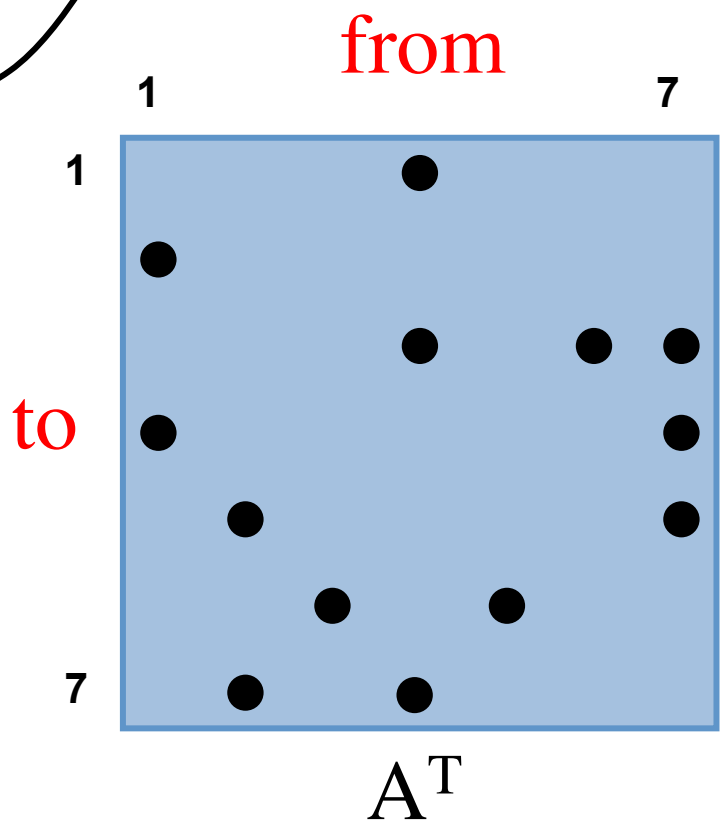


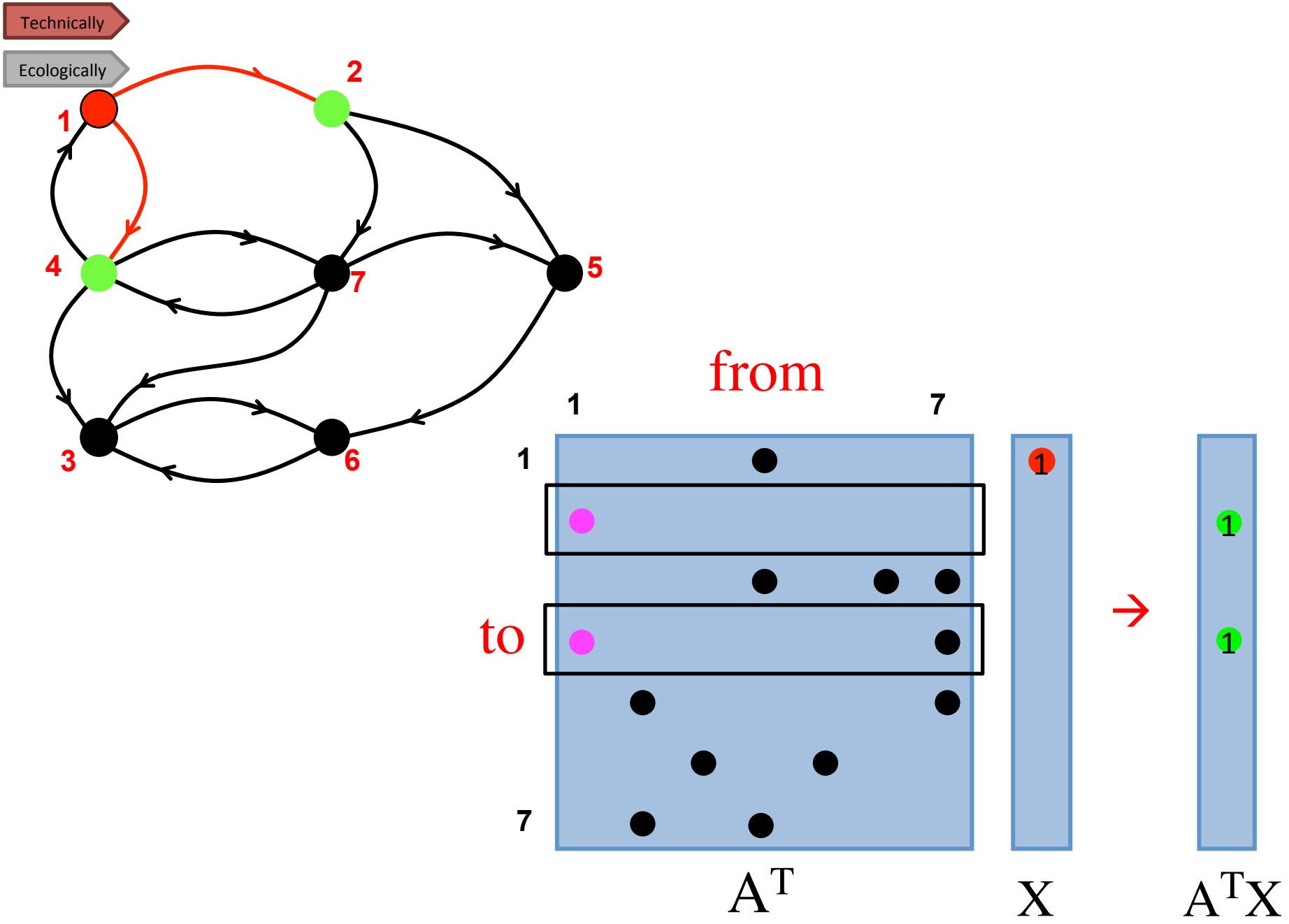
Technically

Ecologically



Example Implementation: bfsTree

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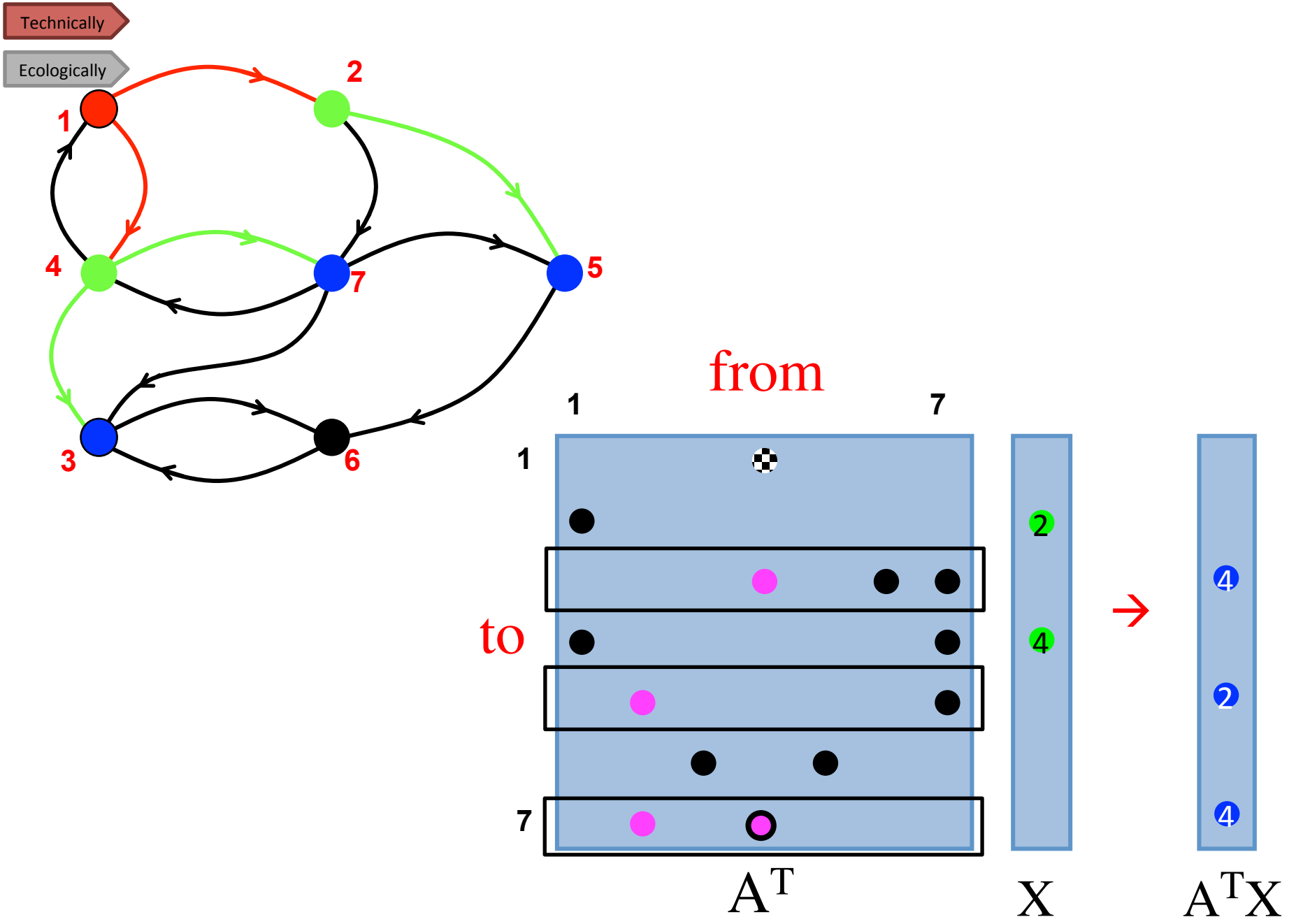
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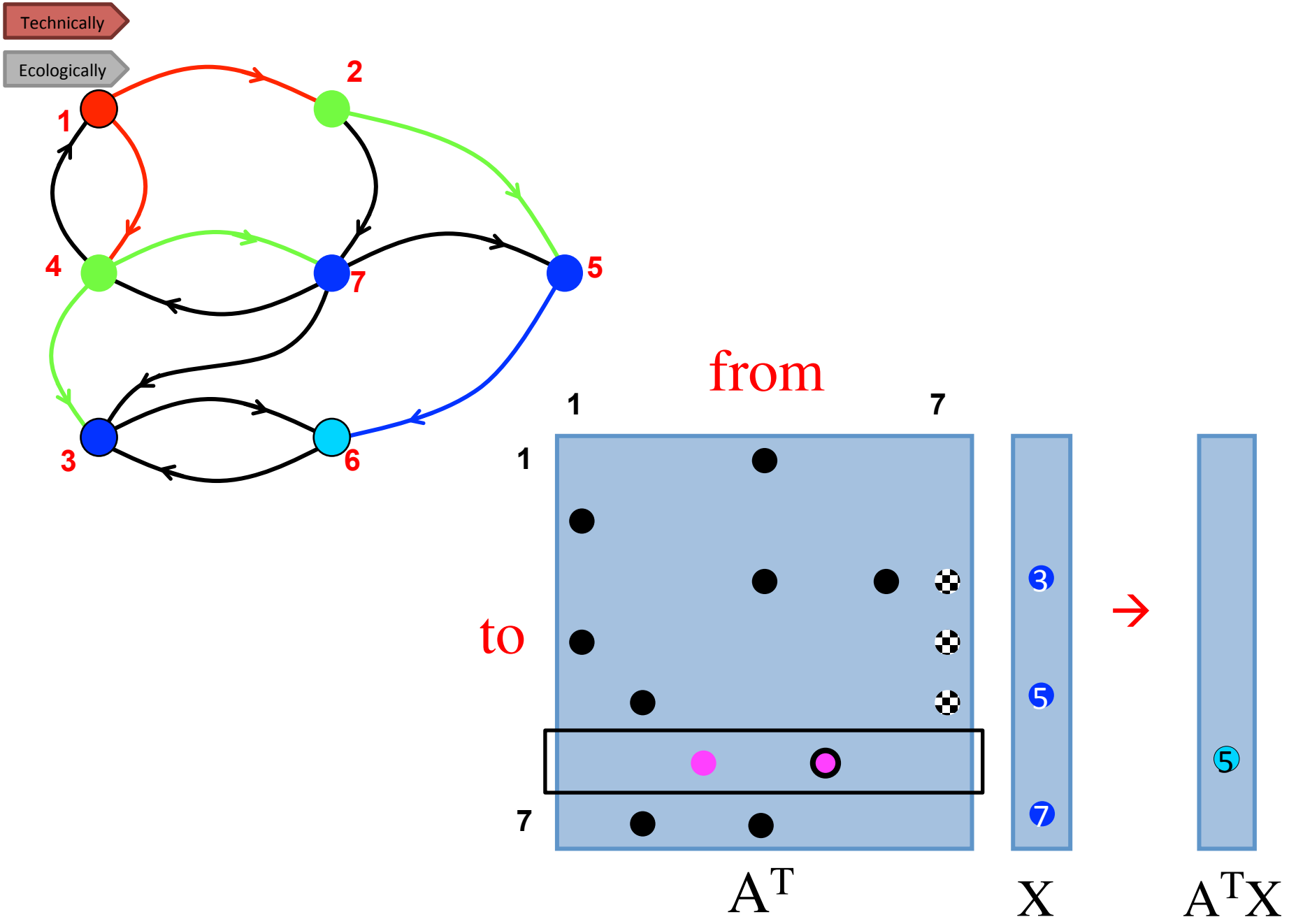
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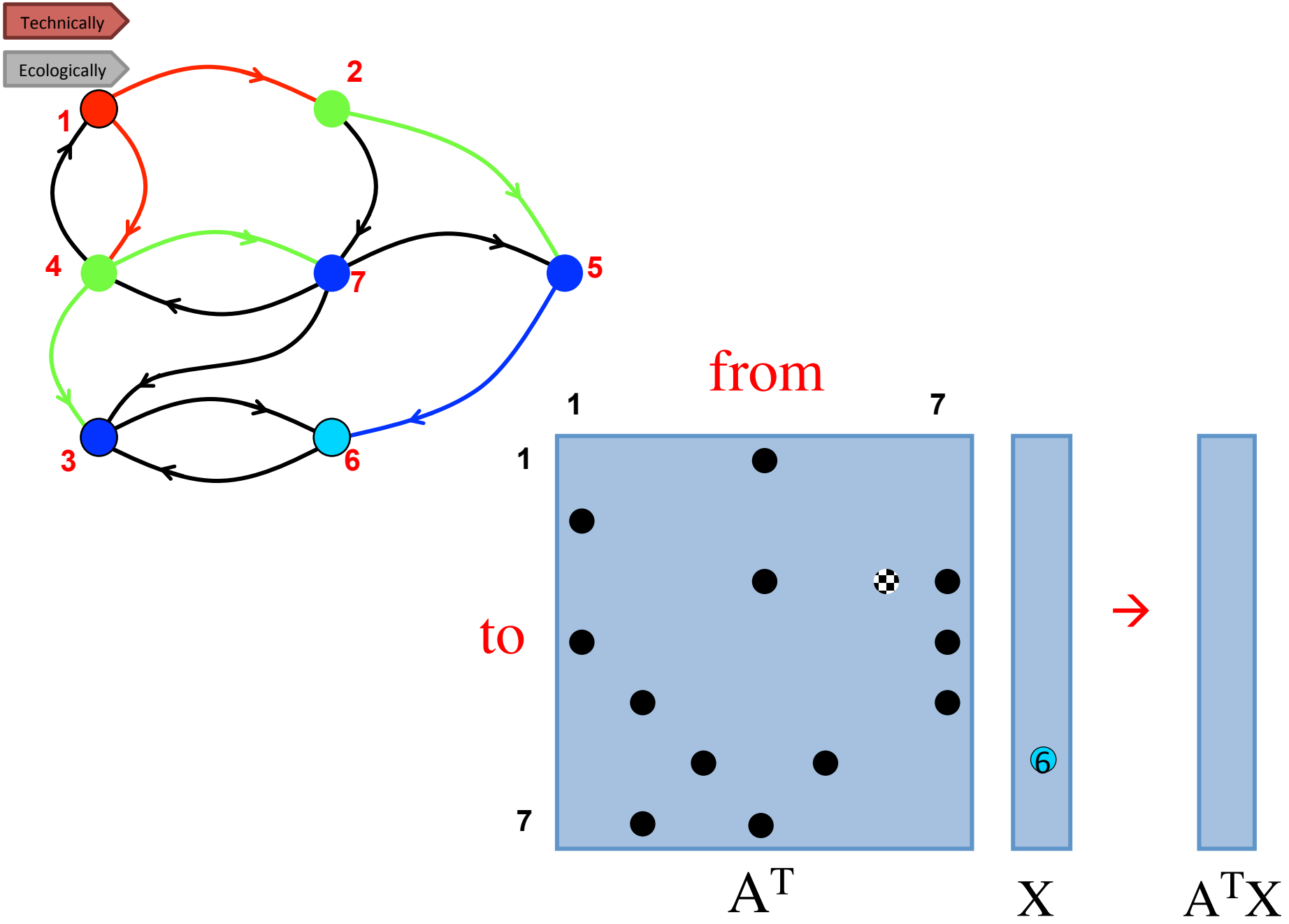
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bfsTree Implementation in KDT, for DiGraphs

(Kernel 2 of Graph500)

Technically

Ecologically

```
def bfsTree(self, root, sym=False):
    if not sym:
        self.T()      # synonym for reverseEdges
    parents = dg.ParVec(self.nvert(), -1)
    fringe = dg.SpParVec(self.nvert())
    parents[root] = root
    fringe[root] = root
    while fringe.nnn() > 0:
        fringe.spRange()
        self._spm.SpMV_SelMax_inplace(fringe._spv)
        pcb.EWiseMult_inplacefirst(fringe._spv,
            parents._dpv, True, -1)
        parents[fringe] = fringe
    if not sym:
        self.T()
    return parents
```

- SpMV and EWiseMult are CombBLAS ops that do not yet have good graph abstractions
  - pathsHop is an attempt for one flavor of SpMV

pageRank Implementation in KDT (p. 1 of 2)

Technically

Ecologically

```
def pageRank(self, epsilon = 0.1, dampingFactor = 0.85):
        # We don't want to modify the user's graph.
        G = self.copy()
        nvert = G.nvert()

        G._spm.removeSelfLoops()

        # Handle sink nodes (nodes with no outgoing edges) by
        # connecting them to all other nodes.
        degout = G.degree(gr.Out)
        nonSinkNodes = degout.findInds()
        nSinkNodes = nvert - len(nonSinkNodes)
        iInd = ParVec(nSinkNodes*(nvert))
        jInd = ParVec(nSinkNodes*(nvert))
        wInd = ParVec(nSinkNodes*(nvert), 1)
        sinkSuppInd = 0

        for ind in range(nvert):
            if degout[ind] == 0:
                # Connect to all nodes.
                for sInd in range(nvert):
                    iInd[sinkSuppInd] = sInd
                    jInd[sinkSuppInd] = ind
                    sinkSuppInd = sinkSuppInd + 1
        sinkMat = pcb.pySpParMat(nvert, nvert,
                        iInd._dpv, jInd._dpv,    wInd._dpv)
        sinkG = DiGraph()
        sinkG._spm = sinkMat
```

- This portion looks more like graph operations

pageRank Implementation in KDT (p. 2 of 2) (main loop)

Technically

Ecologically

```
G.normalizeEdgeWeights()
sinkG.normalizeEdgeWeights()

# PageRank loop
delta = 1
dv1 = ParVec(nvert, 1./nvert)
v1 = dv1.toSpParVec()
prevV = SpParVec(nvert)
dampingVec = SpParVec.ones(nvert) *
                 ((1 - dampingFactor)/nvert)
while delta > epsilon:
    prevV = v1.copy()
    v2 = G._spm.SpMV_PlusTimes(v1._spv) + \
             sinkG._spm.SpMV_PlusTimes(v1._spv)
    v1._spv = v2
    v1 = v1*dampingFactor + dampingVec
    delta = (v1 - prevV)._spv.Reduce(pcb.plus(),
                pcb.abs())
return v1
```

- This portion looks much more like matrix algebra

Graph500 Implementation in KDT (p. 1 of 2)

Technically

Ecologically

```
scale = 15
nstarts = 640

GRAPH500 = 1
if GRAPH500 == 1:
        G = dg.DiGraph()
        K1elapsed = G.genGraph500Edges(scale)

        if nstarts > G.nvert():
                nstarts = G.nvert()
        deg3verts = (G.degree() > 2).findInds()
        deg3verts.randPerm()
        starts = deg3verts[dg.ParVec.range(nstarts)]

G.toBool()

K2elapsed = 1e-12
K2edges = 0
for start in starts:
        start = int(start)
        if start==0:    #HACK:  avoid root==0 bugs for now
                continue
        before = time.time()
        parents = G.bfsTree(start, sym=True)
        K2elapsed += time.time() - before
        if not k2Validate(G, start, parents):
                print "Invalid BFS tree generated by bfsTree"
                print G, parents
                break
        [origI, origJ, ign] = G.toParVec()
        K2edges += len((parents[origI] != -1).find())
```

Graph500 Implementation in KDT (p. 2 of 2)

Technically

Ecologically

```
def k2Validate(G, start, parents):
    ret = True
    bfsRet = G.isBfsTree(start, parents)
    if type(ret) != tuple:
            if dg.master():
                    print "isBfsTree detected failure of Graph500 test %d" % abs(ret)
            return False
    (valid, levels) = bfsRet

    # Spec test #3:
    [origI, origJ, ign] = G.toParVec()
    li = levels[origI]
    lj = levels[origJ]
    if not ((abs(li-lj) <= 1) | ((li==-1) & (lj==-1))).all():
            if dg.master():
                print "At least one graph edge has endpoints whose levels differ by
                            more than one and is in the BFS tree"
            print li, lj
            ret = False

    # Spec test #4:
    neither_in = (li == -1) & (lj == -1)
    both_in = (li > -1) & (lj > -1)
    out2root = (li == -1) & (origJ == start)
    if not (neither_in | both_in | out2root).all():
            if dg.master():
                print "The tree does not span the connected component exactly, root=%d" %
                          start
            ret = False

    # Spec test #5:
    respects = abs(li-lj) <= 1
    if not (neither_in | respects).all():
            if dg.master():
                print "At least one vertex and its parent are not joined by an
                           original edge"
            ret = False

    return ret
```

- #1 and #2: implemented in isBfsTree

- #3: every input edge has vertices whose levels differ by no more than 1. Note: don't actually have input edges, will use the edges in the resulting graph as a proxy

- #4: the BFS tree spans a connected component's vertices (== all edges either have both endpoints in the tree or not in the tree, or source is not in tree and destination is the root)

- #5: a vertex and its parent are joined by an edge of the original graph

isBfsTree implementation KDT (p. 1 of 2)

Technically

Ecologically

```
def isBfsTree(self, root, parents, sym=False):
        ret = 1         # assume valid
        nvertG = self.nvert()

        # calculate level in the tree for each vertex; root is at level 0
        if not sym:
                self.reverseEdges()
        parents2 = ParVec.zeros(nvertG) - 1
        parents2[root] = root
        fringe = SpParVec(nvertG)
        fringe[root] = root
        levels = ParVec.zeros(nvertG) - 1
        levels[root] = 0

        level = 1
        while fringe.nnn() > 0:
                fringe.spRange()
                #ToDo:  create PCB graph-level op
                self._spm.SpMV_SelMax_inplace(fringe._spv)
                #ToDo:  create PCB graph-level op
                pcb.EWiseMult_inplacefirst(fringe._spv, parents2._dpv, True, -1)
                parents2[fringe] = fringe
                levels[fringe] = level
                level += 1
        if not sym:
                self.reverseEdges()
```

isBfsTree implementation KDT (p. 2 of 2)

Technically

Ecologically

```
# build a new graph from just tree edges
tmp2 = parents != ParVec.range(nvertG)
treeEdges = (parents != -1) & tmp2
treeI = parents[treeEdges.findInds()]
treeJ = ParVec.range(nvertG)[treeEdges.findInds()]
if (treeJ == root).any():
    return -1
# note treeJ/TreeI reversed, so builtGT is transpose, as needed by SpMV
builtGT = DiGraph(treeJ, treeI, 1, nvertG)
visited = ParVec.zeros(nvertG)
visited[root] = 1
fringe = SpParVec(nvertG)
fringe[root] = root
cycle = False; multiparents = False
while fringe.nnn() > 0 and not cycle and not multiparents:
        fringe.spOnes()
        newfringe = SpParVec.toSpParVec( builtGT._spm.SpMV_PlusTimes(fringe._spv))
        if visited[newfringe.toParVec().findInds()].any():
                cycle = True
                break
        if (newfringe > 1).any():
                multiparents = True
        fringe = newfringe
        visited[fringe] = 1
if cycle or multiparents:
        return -1

# spec test #2
if (levels[treeI]-levels[treeJ] != -1).any():
         return -2

return (ret, levels)
```

- #1: validate that the tree is a tree and has no cycles:
  - a) no edge has the root as a destination
  - b) no cycle exists
  - c) no vertex has more than 1 parent
- #2: tree edges should be between vertices whose levels differ by 1