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Computing Hypergraph Homology in Chapel

Jesun Firoz (PNNL)

Louis Jenkins (U Rochester),Cliff Joslyn (PNNL),
Brenda Praggastis (PNNL), Emilie Purvine (PNNL),
Mark Raugas (PNNL)

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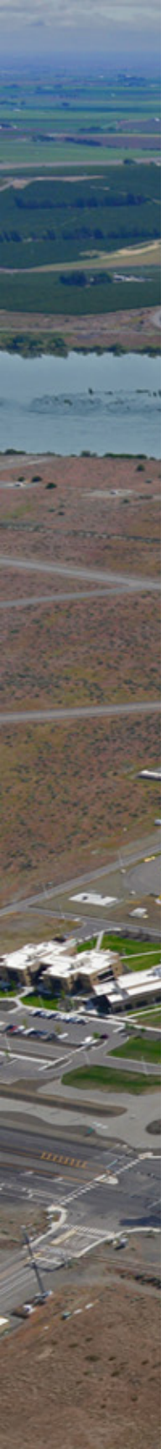

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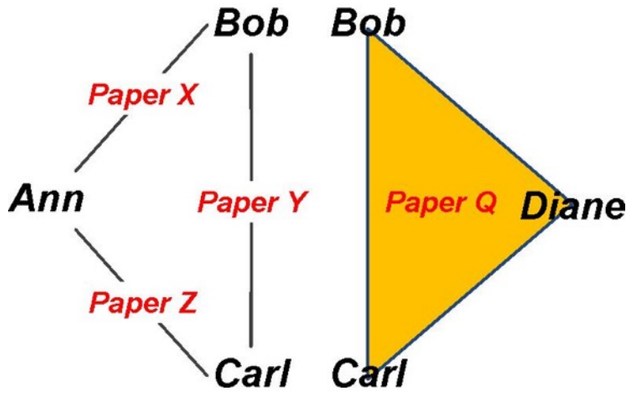
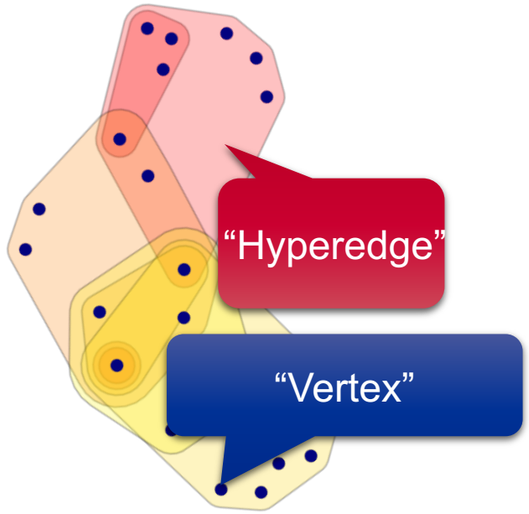
Outline

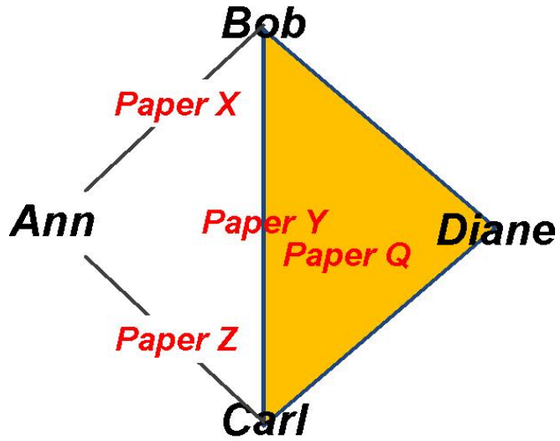
- Hypergraphs
- Hypergraph Homology Computation
  - Motivation
- Linear algebra operations: Chapel vs Python
- Hypergraph Homology Computation in Chapel
  - Two main steps
  - Optimizations
  - Experimental results

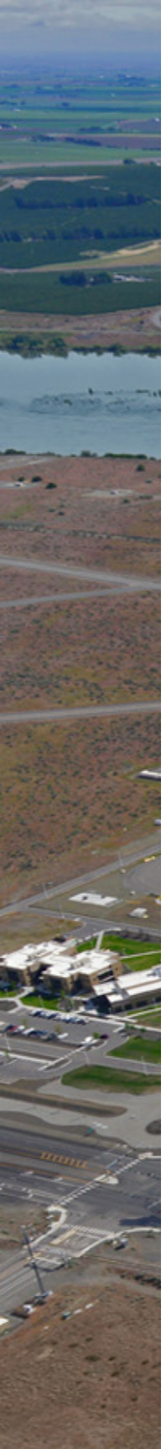
Hypergraphs

- **Graphs** model distributed interactions among entities
  - Questions of connectivity, reachability, density, clustering
- ***But multi-way interactions cannot be modeled natively by graphs!***
  - **Requires higher coding strategies:** Property graphs, reification, bipartite structures
- **Multi-Dimensional Graph:** Hypergraph









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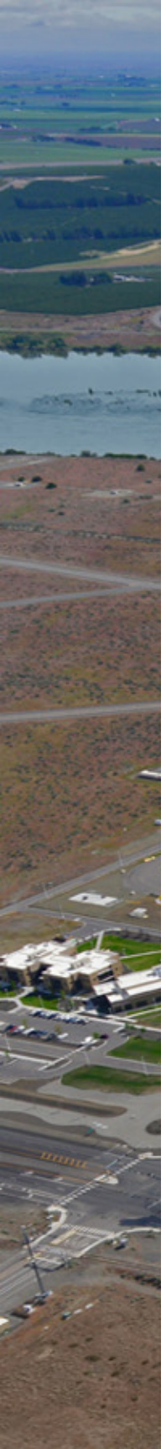
Hypergraph Homology Computation in Chapel

- Motivation:
  - Learn about missing data and their surrounding datasets.
  - Datasets and ASCs can be huge.
  - Leverage Chapel's parallel and distributed execution capability to run at scale.
- Two main steps:
  - Computing the boundary matrices
  - Computing the Smith Normal form of a matrix.
- Heavily involves matrix and linear algebra operations.



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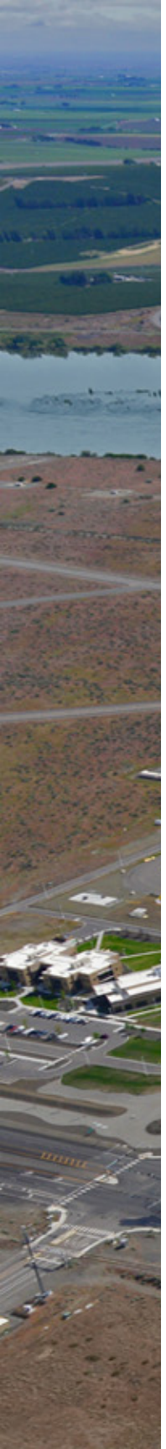
Homology Computation in Chapel (Cont.)

- Matrices are represented as 2D arrays in Chapel.
- Array-centric operations include:
  - Row and column interchange,
  - Pivot calculation,
  - Addition of rows and columns,
  - Rank computation,
  - Multiplication, and
  - Slicing
- In Chapel, such operations are very concise and more intuitive than in Python.
- While Chapel's linear algebra library performs various operations on matrices (such as singular value decomposition, LU decomposition etc.), our operations are in the Z_2 field, so we wrote our own.



Linear Algebra Operations: Chapel vs Python

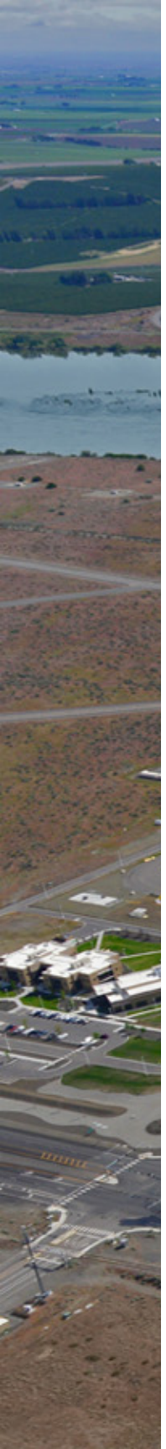
Chapel

```
1  proc swap_rows(i,j,M) {
2    var N = M;
3    N[i, ..] <=> N[j, ..];
4    return N;
5  }
6  proc add_to_row(M,i,j,ri=1,rj=1) {
7    var N = M;
8    N[i, ..]  = (ri * N[i, ..] + rj * N[j, ..]) % 2;
9    return N;
10 }
11 proc calculateRank(M) return + reduce
12   [i in M.domain.dim(2)] (max reduce M[.., i]);
```

Python (Numpy/sequential)

```
1  def rowswap(i,j,M):
2  N = copy.deepcopy(M)
3      N[i] = M[j]
4      N[j] = M[i]
5      return N
6  def add_to_row(M,i,j,ri=1,rj=1,mod=2):
7      N = copy.deepcopy(M)
8      N[i] = np.mod(ri*N[i] + rj*N[j],[mod])
9      return N
10 def calculaterank(M):
11   return np.sum(M)
```

Reduction intent: For each column, see if at least one 1, **in parallel**



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Linear Algebra Operations: Chapel vs Python

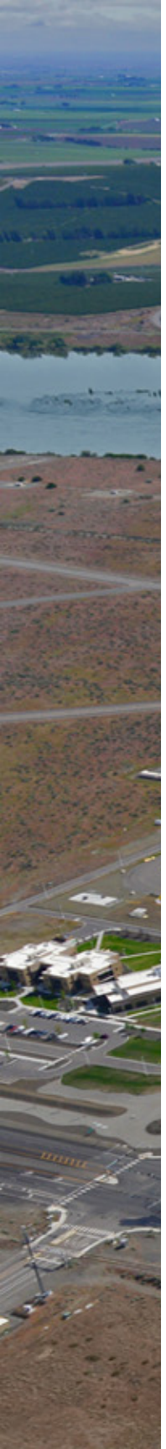
Chapel

```chapel
proc matmultmod (M, N, mod =2) {
  var C : [M.domain.dim(1), N.domain.dim(2)] int;
  forall (i,j) in C.domain {
    C[i,j] = (+ reduce (M[i, M.domain.dim(2)]
     * N[M.domain.dim(2), j])) % 2;
  return C;
}
```

Parallel matrix multiplication

Python (Numpy/sequential)

```python
def modmult(M,N,mod=2):
  return np.mod(np.matmul(M,N),mod)
```



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Homology Computation in Chapel

Step 1. Boundary Matrix Computation: What We Will Do

- For example: Given a hypergraph with one hyperedge with four vertices:

```
1 [{ 0  1  2  3 }]
```

- Generate the ASCs (powerset of the hyperedge) and accumulate the k-cells in the corresponding bins:

```
1 2 -> [{ 0  1  2 }, { 0  1  3 }, { 0  2  3 }, { 1  2  3 }]
2 1 -> [{ 0  1 }, { 0  2 }, { 0  3 }, { 1  2 }, { 1  3 }, { 2  3 }]
3 0 -> [{ 0 }, { 1 }, { 2 }, { 3 }]
4 3 -> [{ 0  1  2  3 }]
```

0-cells

- Compute the boundary maps:

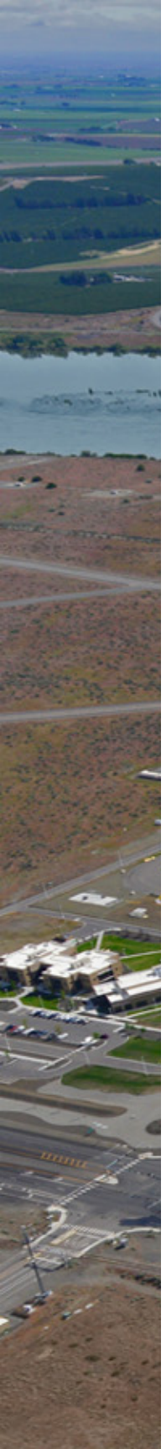
1-cells

0-cells

	1	2	3	4	5	6
1	1	1	1	0	0	0
2	1	0	0	1	1	0
3	0	1	0	1	0	1
4	0	0	1	0	1	1

	1	2	3	4
1	1	1	0	0
2	1	0	1	0
3	0	1	1	0
4	1	0	0	1
5	0	1	0	1
6	0	0	1	1

	1
1	1
2	1
3	1
4	1



Boundary Matrix Computation
Step 1a: Computing Abstract Simplicial Cell Complexes (ASCs)

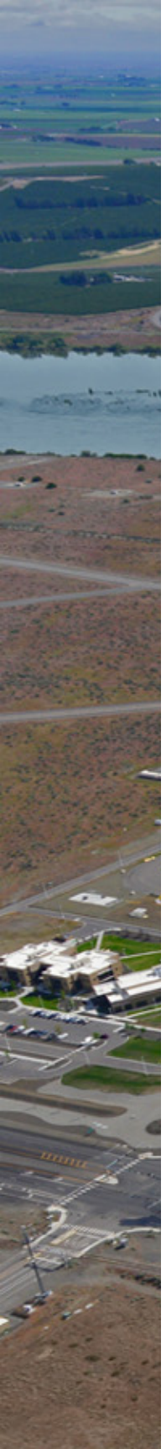
Maintain one set per task per locale for gathering the ASCs

```
1 var cellSets : [0..#numLocales, 0..#here.maxTaskPar] set(Cell);
```

Each edge computes the ASCs in parallel

```
1 var taskIdCounts : [0..#numLocales] atomic int;
2 forall e in hypergraph.getEdges()
3   with (var tid : int = taskIdCounts[here.id].fetchAdd(1)) {
4   var vertices = hypergraph.incidence(e);
5   ref tmp = vertices[1..#vertices.size];
6   var verticesInEdge : [1..#vertices.size] int = tmp.id;
7   processCell(new Cell(verticesInEdge), cellSets[here.id, tid]);
8 }
```

Generate power set/ASCs for the hyperedge



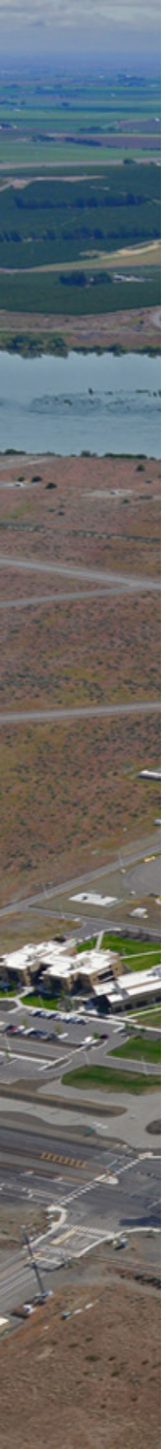
Boundary Matrix Computation
Step 1b: Combining K-cells

```
1 var cellSets : [0..#numLocales, 0..#here.maxTaskPar] set(Cell);
```

Hashed distribution that maps the distributed associative domains of cells to target locales

```
1 var cellSet : domain(Cell, parSafe=true) dmapped Hashed(idxType=Cell);
2 for cset in cellSets {
3   forall cell in cset with (ref cellSet) {
4     cellSet += cell;
5   }
```

Adding cells to the domain



Boundary Matrix Computation
Step 1b: Binning all K-cells

Bin cells based on their sizes

Thread-safe map

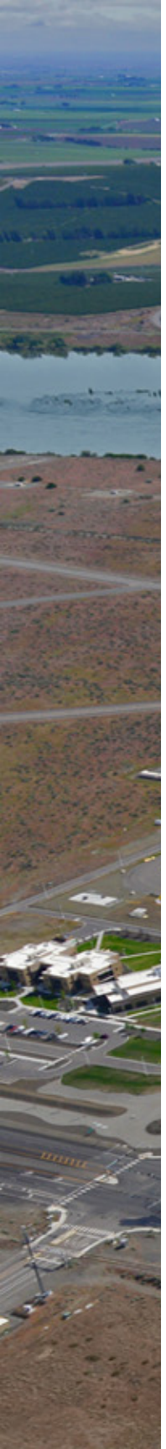
```
1 var kCellMap = new map(int, list(Cell, parSafe=true), parSafe=true);
2 forall cell in cellSet {
3   kCellMap[cell.size - 1].append(cell);
4 }
```

Potential bottleneck: merge is happening on one Locale.

```
1 forall (_kCellsArray, kCellKey) in zip(kCellsArrayMap, kCellKeys){
2   _kCellsArray = new owned kCellsArray(kCellMap[kCellKey].size);
3   _kCellsArray.A = kCellMap[kCellKey].toArray();
4   sort(_kCellsArray.A, comparator=absComparator);
5 }
```

Sort each bin in parallel

Customized comparator for sorting



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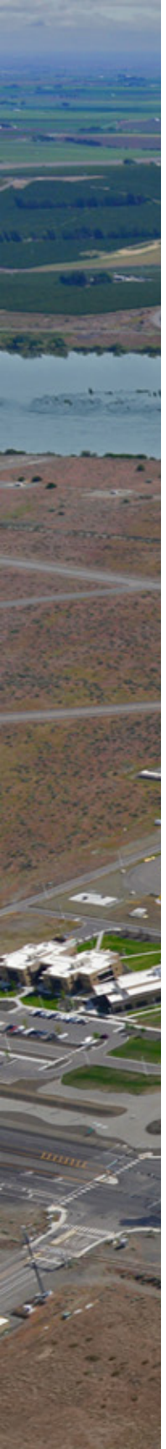
Boundary Matrix Computation: Comparator for Sorting Bins

- Customized comparator for sorting

```
1 proc Comparator.compare(a : Cell, b : Cell) : int {
2   assert(a.size == b.size);
3   for (_a, _b) in zip(a,b) {
4     if (_a > _b) then return 1;
5     else if (_a < _b) then return -1;
6   }
7   return 0;
8 }
```



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Boundary Matrix Computation: What We Have Done So Far

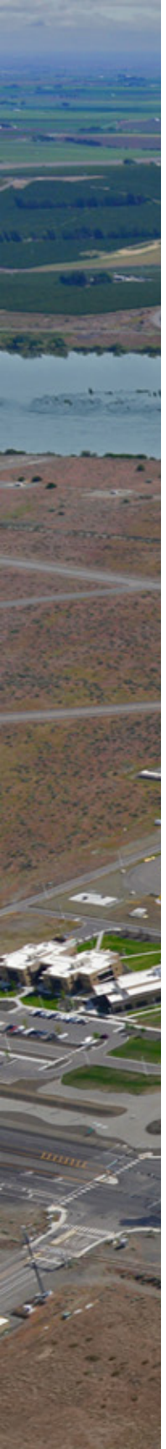
- For example: Given a hypergraph with one hyperedge with four vertices:

```
1 [{ 0  1  2  3 }]
```

- Generate the ASCs (powerset of the hyperedge) and accumulate the k-cells in the corresponding bins:

```
1 2 -> [{ 0  1  2 }, { 0  1  3 }, { 0  2  3 }, { 1  2  3 }]
2 1 -> [{ 0  1 }, { 0  2 }, { 0  3 }, { 1  2 }, { 1  3 }, { 2  3 }]
3 0 -> [{ 0 }, { 1 }, { 2 }, { 3 }]
4 3 -> [{ 0  1  2  3 }]
```

0-cells



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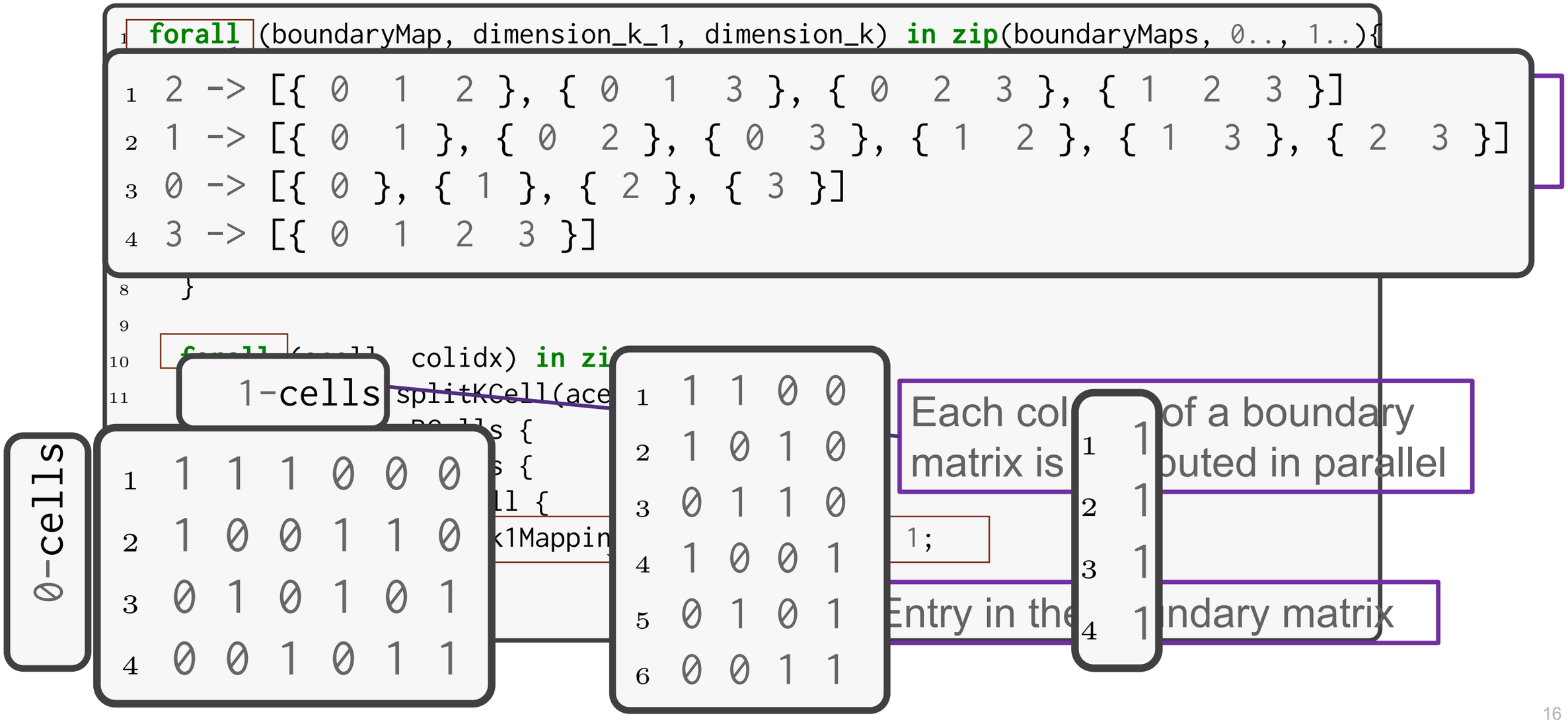
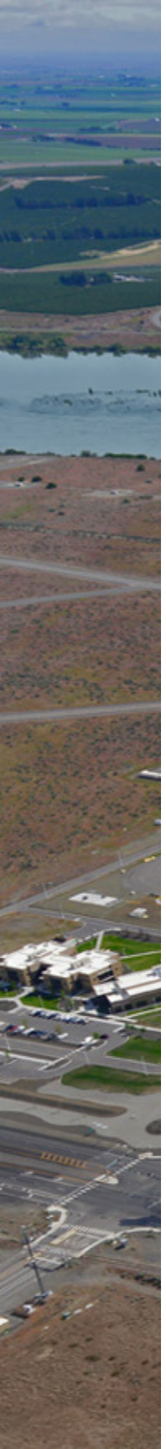
Boundary Matrix Data Structure

```
1 class Matrix {
2   var N : int;
3   var M : int;
4   var D = {1..N, 1..M} dmapped Block(boundingBox = {1..N, 1..M});
5   var matrix : [D] int;
6   proc init(_N: int, _M:int) {
7     N = _N;
8     M = _M;
9 }
```

Block-distributed 2D array

Boundary Matrix Computation





Boundary Matrix Computation: What we have done so far

- Given the bins:

```
2 -> [{ 0  1  2 }, { 0  1  3 }, { 0  2  3 }, { 1  2  3 }]
1 -> [{ 0  1 }, { 0  2 }, { 0  3 }, { 1  2 }, { 1  3 }, { 2  3 }]
0 -> [{ 0 }, { 1 }, { 2 }, { 3 }]
3 -> [{ 0  1  2  3 }]
```

- Computed the boundary maps:

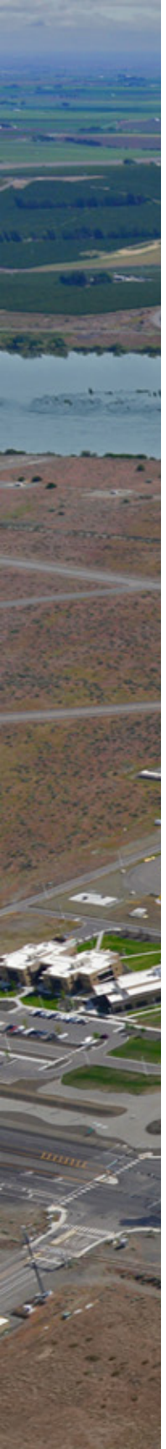
1-cells

0-cells

1	1	1	1	0	0	0
2	1	0	0	1	1	0
3	0	1	0	1	0	1
4	0	0	1	0	1	1

1	1	1	0	0
2	1	0	1	0
3	0	1	1	0
4	1	0	0	1
5	0	1	0	1
6	0	0	1	1

1	1
2	1
3	1
4	1



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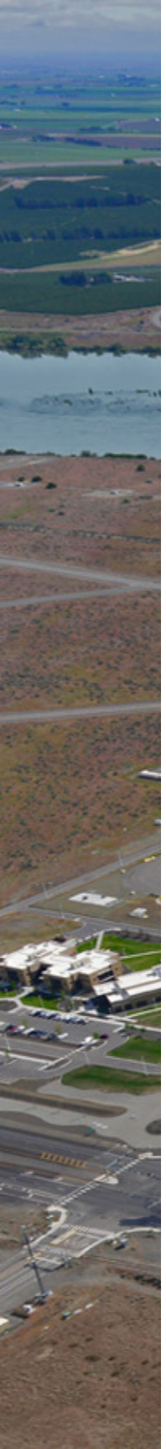
Computing the Smith Normal Form: Recall the Linear Algebra Operations

```
1  proc swap_rows(i, j, M) {
2    var N = M;
3    N[i, ..] <=> N[j, ..];
4    return N;}
5  proc swap_columns(i, j, M) {
6    var N = M;
7    N[.., i] <=> N[.., j];
8    return N;}
9  proc add_to_row(M, i, j, ri = 1, rj = 1, mod = 2) {
10   var N = M;
11   N[i, ..]  = (ri * N[i, ..] + rj * N[j, ..]) % mod;
12   return N;}
13 proc add_to_column(M, i, j, ci = 1, cj = 1, mod = 2) {
14   var N = M;
15   N[.., i]  = (ci * N[.., i] + cj * N[..,j]) % mod;
16   return N;}
```



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Computing the Smith Normal Form: Recall the Linear Algebra Operations (Cont.)

```
1 proc matmultmod (M, N, mod =2) {
2   var C : [M.domain.dim(1), N.domain.dim(2)] int;
3   forall (i,j) in C.domain {
4     C[i,j] = (+ reduce (M[i, M.domain.dim(2)]
5       * N[M.domain.dim(2), j])) % 2;
6   return C;
7 }
```

Each entry in the resultant matrix is computed in parallel

Reduction intent: doing partial multiplications in parallel and then combining the partial sums

Putting it all together for Computing Smith Normal Form with the Basic LA Operations: LbR=S

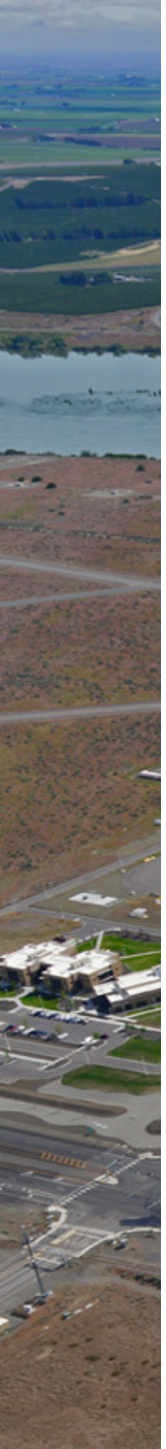
Swapping rows/Columns

```
1  proc smithNormalForm(b) {
2    var IL = IdentityMatrix(dimL);
3    for s in 1..minDim {
4      var pivot = _get_next_pivot(S,s);
5      var rdx : int, cdx : int;
6      (rdx, cdx) = pivot;
7      if (rdx > s) {
8        S = swap_rows(s, rdx, S);
9        L = swap_rows(s, rdx, L);
10       var tmp = swap_rows(s, rdx, IL);
11       var LM = new unmanaged Matrix2D(tmp.domain.high(1),
12                   tmp.domain.high(2));
13       LM._arr = tmp;
14       Linv.append(LM);
15     }
16     if (cdx > s) {
17       S = swap_columns(s, cdx, S);
18       R = swap_columns(s, cdx, R);
19       var tmp = swap_columns(s, cdx, IR);
20       var RM = new unmanaged Matrix2D(tmp.domain.high(1),
21                   tmp.domain.high(2));
22       RM._arr = tmp;
23       Rinv.append(RM);
24     }
```

Potential Bottleneck !!

```
1  proc smithNormalForm(b) {
2  //cont..
3    var row_indices = [idx in 1..dimL]
4           if (idx != s && S(idx,s) == 1) then idx;
5    for rdx in row_indices {
6      S = add_to_row(S, rdx, s);
7      L = add_to_row(L, rdx, s);
8      var tmp = add_to_row(IL, rdx, s);
9      var LM = new unmanaged Matrix2D(tmp.domain.high(1),
10                  tmp.domain.high(2));
11     LM._arr = tmp;
12     Linv.append(LM);
13   }
14   var column_indices = [jdx in 1..dimR]
15          if (jdx != s && S(s,jdx) == 1) then jdx;
16   for (jdx,cdx) in zip(1..,column_indices) {
17     S = add_to_column(S, cdx, s);
18     R = add_to_column(R, cdx, s);
19     var tmp = add_to_column(IR, cdx, s);
20     var RM = new unmanaged Matrix2D(tmp.domain.high(1),
21                  tmp.domain.high(2));
22     RM._arr = tmp;
23     Rinv.append(RM);
24   }
25 }
26 var LinvF = matmulreduce(Linv);
27 var RinvF = matmulreduce(Rinv, true, 2);
28 return (L,R,S,LinvF,RinvF);}
```

Adding to rows/Columns



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Opportunities for parallelization

- Straightforward: Compute SNF of all the boundary matrices in parallel.

```
1 var computedMatrices = smithNormalForm(boundaryMaps[1].matrix);
```

- Interesting case: Multiplying a list of matrices in parallel.

```
1  type listType = list(unmanaged Matrix?, true);
2  proc matmulreduce(arr : listType, reverse = false, mod = 2) {
3    var PD = arr[if reverse then arr.size else 1].D;
4    var P : [PD] int;
5    P = arr(1).matrix;
6    for i in 2..arr.size {
7      ref temp = matmultmod(P, arr(i).matrix);
8      PD = temp.domain;
9      P = temp;
10 }}
```

List of matrices to be multiplied

Pairwise matrix multiplication

- Reminder: What are these matrices? All the intermediate transformations done on a boundary matrix
  - Depending on the number of transformation, list-size may vary

Profiling Result

chplvis

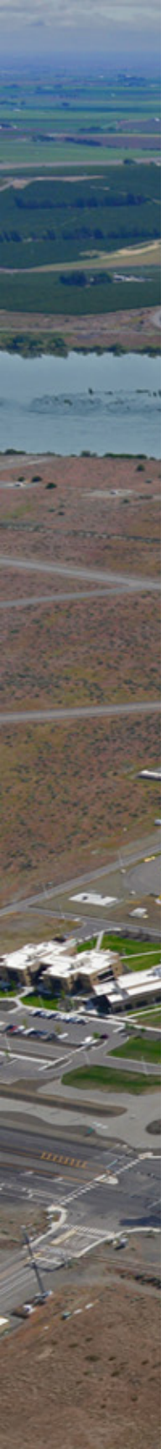
file: SNF

Clock	Internal Function Name	File:line
418.9617	wrapcoforall_fn_chpl154	betti_number_calculator_parallel.chpl:516
31.4294	wrapcobegin_fn31	modules/internal/ChapelArray.chpl:302
30.6619	wrapcobegin_fn34	modules/internal/ChapelArray.chpl:305
27.5633	wrapcoforall_fn_chpl8	modules/dists/BlockDist.chpl:890
27.3298	wrapcoforall_fn_chpl5	modules/dists/BlockDist.chpl:884
26.8153	wrapcoforall_fn_chpl9	modules/dists/BlockDist.chpl:898
15.5744	wrapcoforall_fn_chpl157	betti_number_calculator_parallel.chpl:517
0.0505	wrapcoforall_fn_chpl159	betti_number_calculator_parallel.chpl:547
0.0338	wrapcoforall_fn40	modules/internal/ChapelArray.chpl:4171
0.0228	wrapcoforall_fn30	modules/internal/ChapelArray.chpl:4171

```
proc matmultmod (M, N, mod =2) {
  var CD = {M.domain.dim(1), N.domain.dim(2)} dmapped Block(boundingBox = {M.domain.dim(1), N.domain.dim(2)});
  var C : [CD] int;
  forall (i,j) in C.domain {
    C[i,j] = (+ reduce (M[i, M.domain.dim(2)] * N[M.domain.dim(2), j])) % 2;
  }
  return C;
}
```

- Matrix multiplication is the bottleneck.
- Shared-memory vs distributed 2D array →lots of associated overhead

- In one of the test cases, with 20 vertices and 20 hyperedges, on one compute node/ 1 locale with InfiniBand interconnect and 20-cores, sequential execution took 25s vs distributed-memory 2D version took ~2400s !!



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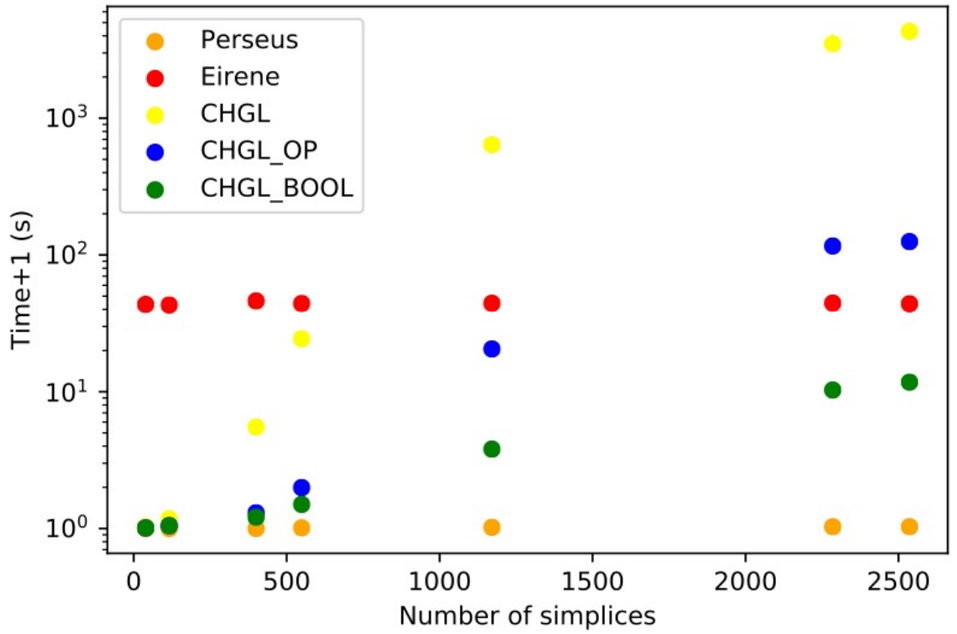
Algorithmic Optimizations

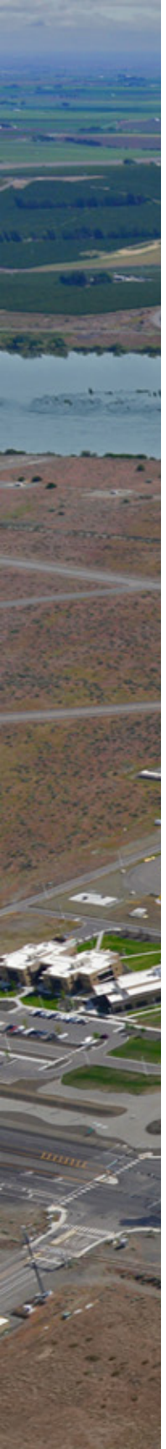
- Optimization 1: Reformulated the calculation of Smith Normal Form
  - Eliminate the requirement of performing explicit matrix-multiplications.
  - Instead, in-place modification of the matrices are made on-the-fly to find the invertible matrices.
- Optimization 2: Since all of our computations are done in the Z_2 field,
  - Opted for boolean datatype and operations for boundary matrices instead of integer matrices.
  - Accordingly, some of the matrix operations changed: for example add_to_row operation on Boolean matrix is elementwise xor.

Experimental Result

- Platform: A single compute node with a 20-core Intel Xeon processor and 132GB memory.
- Chapel version 1.20
- Compared with two other homology packages: Perseus (writtenin C++) and Eirene (written in Julia).



Legends:
CHGL: with explicit matmult
CHGL_OP: No explicit matmult
CHGL_BOOL: Boolean datatype



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Conclusion and Future Plan

- Implemented parallel/distributed homology computation in CHGL
  - Computing the boundary matrix
  - Computing the Smith normal form (SNF) of matrices
  - Computing the reduced row Echelon form (Not shown here, similar to SNF)
- Linear algebra operations in the homology computation in Chapel
  - Concise
  - Intuitive
  - Parallel and distributed
- Bottlenecks:
  - Overhead of shared-memory vs block-distributed 2D arrays.
  - Matrix multiplication is one of the main time-consuming kernel
  - Multiplications of list of matrices need to be done in parallel.
- **Moving forward:**
  - Scalable and efficient Parallel/distributed implementation (Ongoing) and scaling test

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Thank you