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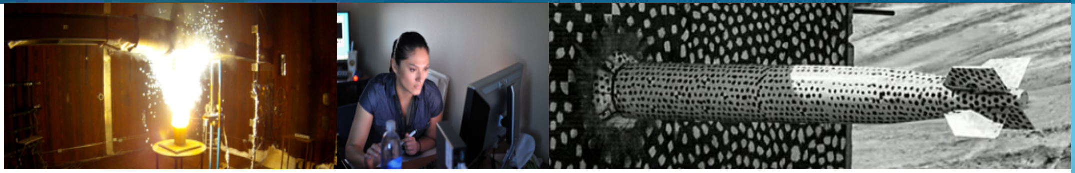
Parallel Graph Partitioning and Randomized Linear Algebra



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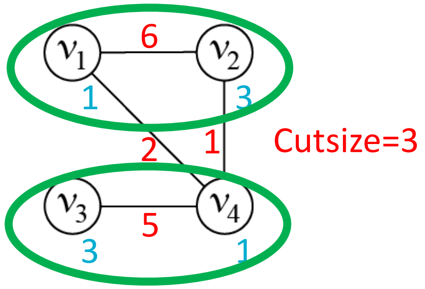
U.S. DEPARTMENT OF ENERGY NNSA

Sphynx – Highlights

- Sphynx: Spectral Partitioning for HYbrid aNd aXelarator-based systems
- Sphynx uses several Trilinos packages using Kokkos for performance portability
- Sphynx is the first multi-GPU partitioner for distributed-memory systems
- Compared to ParMETIS, Sphynx is faster on irregular graphs and obtains similar quality partitions on regular graphs

Sphynx – Problem Statement

- Graph $G = (V, E)$: set of vertices V, set of edges E
- For the graph partitioning problem
  - each vertex is assigned a weight value
  - each edge is assigned a cost value



- A K-way partition Π of G
  - is balanced if there is a balance on part weights
  - has a cutsize defined as the sum of the cut-edge costs
- Graph partitioning problem is to find a balanced K-way partition of G with minimum cutsize

Sphynx – Motivation

- We are revisiting graph partitioning problem, because:
  - Applications are moving to accelerators
  - DoE facilities have announced different accelerators
    - AMD, Intel, NVIDIA GPUs
  - No accelerator-enabled graph partitioning tool exists
  - We provide Sphynx to fill this gap
    - Distributed-memory parallel, accelerator-enabled, and portable
- Sphynx is based on a spectral approach, because:
  - Spectral methods use linear-algebra kernels, which are more amenable to parallelization on accelerators
  - Can potentially speed up algorithm with randomized linear algebra

Background: Spectral partitioning

- Proposed by Pothen, Simon, Liou (1989-90)
- Eigenvalue problems: combinatorial, generalized, and normalized
- Adjacency matrix $A = (a)_{ij} = \begin{cases} 1 & \text{if } e_{i,j} \in E \\ 0 & \text{otherwise} \end{cases}$
- Degree matrix $D = (d)_{ij} = \begin{cases} \deg(v_i) & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$
- Form a Laplacian matrix:
  - Combinatorial Laplacian $L_C = D - A$
  - Normalized Laplacian $L_N = I - D^{-1/2} A D^{-1/2}$
- Find eigenvectors x corresponding to smallest nontrivial eigenvalues $\lambda > 0$ s.t.
  - $L_C x = \lambda x$, for combinatorial eigenvalue problem
  - $L_C x = D \lambda x$, for generalized eigenvalue problem
  - $L_N x = \lambda x$, for normalized eigenvalue problem

Why Revisit Spectral Methods Now?

Weren't they abandoned in the '90s and replaced by multilevel methods? Yes, but…

- Quality of spectral partitioners are often only slightly worse than multilevel.
- Preconditioned eigensolvers (LOBPCG) came later.
- Linear algebra operations have been optimized for GPU.
- Spectral partitioning is robust for large #proc (#GPU), as eigenvectors don't change

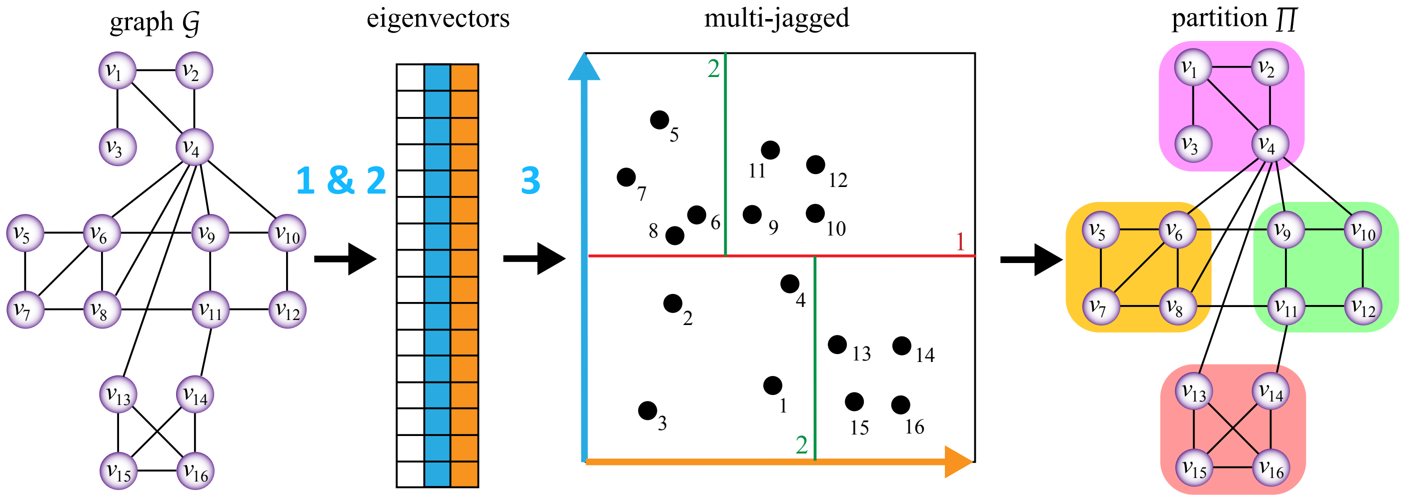
Sphynx – Spectral partitioning

- Traditional spectral methods [1] use recursive bipartitioning. At each bipartitioning step, they
  - compute one eigenvector (Fiedler vector) on the current graph
  - sort the vertices w.r.t. the entries of the eigenvector
  - bipartition the vertices according to the sorted order
- Sphynx computes $(\log K + 1)$ eigenvectors of the Laplacian, all at once
- Computing all eigenvectors at once avoids
  - forming subgraphs and/or corresponding Laplacians
  - moving subgraphs across different processes
  - calling eigensolver multiple times

[1] A. Pothen, H. Simon, and K. Liou, "Partitioning sparse matrices with eigenvectors of graphs," SIAM J. Matrix Anal., vol. 11, pp. 430–452, July 1990.

Sphynx – Trilinos framework

1. Create Laplacian L for G – **Tpetra** CrsMatrix, **Kokkos** parallel_for
2. Compute $(\log K + 1)$ eigenvectors of L using LOBPCG [1] – ***Anasazi***
   - First eigenvector: trivial, not used
   - Remaining vectors: coordinates to embed G into $\log K$-dimensional space
3. Compute a K-way partition on coordinates using multi-jagged [2] – ***Zoltan2***


graph G
eigenvectors
multi-jagged
partition Π
1 & 2
3
v_1 v_2 v_3 v_4 v_5 v_6 v_7 v_8 v_9 v_{10} v_{11} v_{12} v_{13} v_{14} v_{15} v_{16}
1
2
2

[1] A. V. Knyazev,"Toward the optimal preconditioned eigensolver: Locally optimal block preconditioned conjugate gradient method," SIAM Journal on Scientific Computing, vol. 23, no. 2, pp. 517–541, 2001.

[2] M. Deveci, S. Rajamanickam, K. D. Devine, and U. V. Catalyurek, "Multi-jagged: A scalable parallel spatial partitioning algorithm," IEEE Transactions on Parallel and Distributed Systems, vol. 27, pp. 803–817, March 2016.

Sphynx – Preconditioning

- Number of iterations in LOBPCG is a bottleneck
- LOBPCG allows using a preconditioner
- Sphynx supports three preconditioners

1. Jacobi: $M = diag(A)^{-1}$ **(Ifpack2)**
   - scaling each row by the inverse of the diagonal, easy to parallelize
2. Polynomial: $M = p_k(A)$ **(Belos)**
   - SpMV to apply, highly parallel
   - based on GMRES polynomial
3. (Algebraic) Multigrid: $A_{\ell+1} = RA_\ell P$ **(MueLu)**
   - multilevel, captures more global information
   - costlier setup

Sphynx – Experiments

- The GPU focus: MPI+Kokkos (Cuda/HIP)
- Performed on Summit and used 24 GPUs
  - Desired number of parts = K = 24
- Each GPU is exclusively used by one MPI rank (default)
- Device allocations in the Unified Virtual Memory (default)
- Initial distribution of the test graphs: 1D block
  - This is the default distribution with Tpetra CrsMatrix
- Parameter sensitivity and comparison against the state of the art
  - Performance metrics: cutsize and runtime

Sphynx – Dataset

	graph	#vertices	#edges	degree	
				max	avg
regular	ecology1	1,000,000	4,996,000	5	5
	dielFilterV2real	1,157,456	48,538,952	110	42
	thermal2	1,227,087	8,579,355	11	7
	Bump_2911	2,852,430	127,670,910	195	45
	Queen_4147	4,147,110	329,499,284	81	79
	100^3	1,000,000	26,463,592	27	26
	200^3	8,000,000	213,847,192	27	27
	400^3	64,000,000	1,719,374,392	27	27
irregular	hollywood-2009	1,069,126	113,682,432	11,468	106
	com-Orkut	3,072,441	237,442,607	33,314	77
	wikipedia-20070206	3,512,462	88,261,228	187,672	25
	cit-Patents	3,764,117	36,787,597	794	10
	com-LiveJournal	3,997,962	73,360,340	14,816	18
	wb-edu	8,863,287	97,233,789	25,782	11
	uk-2005	39,252,879	1,602,132,663	1,776,859	41
	it-2004	41,290,577	2,096,240,367	1,326,745	51
	twitter7	41,652,230	2,446,678,322	2,997,488	59
	com-Friendster	65,608,366	3,677,742,636	5,215	56
	FullChip	2,986,914	26,621,906	2,312,481	9
	circuit5M	5,555,791	59,519,031	1,290,501	11

The SuiteSparse Matrix Collection, https://sparse.tamu.edu/

Sphynx – Results

- Comparison against ParMETIS [1] and XtraPuLP [2]
  - ParMETIS and XtraPuLP **do not run** on GPUs
- Application-friendly comparison on 24 MPI ranks
  - Sphynx uses 6 MPI ranks per node and 1 GPU per rank
  - ParMETIS uses 6 MPI ranks per node
  - XtraPuLP uses 6 MPI ranks per node and 7 OpenMP threads per rank

Average results normalized w.r.t Sphynx

	ParMETIS		XtraPuLP	
	runtime	cutsize	runtime	cutsize
regular	0.33	0.81	0.31	6.36
irregular	23.95	0.30	1.24	0.45

- ParMETIS execution **did not finish** in 2 hours on 4 graphs
  - Largest irregular graphs: uk-2005, it-2004, twitter7, com-Friendster

[1] G. Karypis, V. Kumar, Parmetis: Parallel graph partitioning and sparse matrix ordering library, Tech. rep., Dept. Computer Science, University of Minnesota, 1997.
[2] G. M. Slota, S. Rajamanickam, K. Devine, K. Madduri, Partitioning trillion-edge graphs in minutes, IPDPS, 2017.

Randomized Eigensolvers

- The most expensive phase (90-95%) in spectral partitioning is the eigensolver
- Fairly low accuracy is sufficient to obtain good partitioning
- Key idea: We can use a randomized eigensolver instead of LOBPCG
  - Randomized methods often get low-accuracy solutions very fast
  - We follow the approach in Halko, Martinsson, Tropp (20XX)
- We have explored this approach in a prototype
  - HPC implementation in Trilinos/Sphynx still to do

Randomized Method: Phase I

- Here we will use the normalized Laplacian, L_N
  - We estimate the largest eigenvalues of the normalized adjacency matrix, which correspond to the smallest eigenvalues of L_N
- First, we approximate the range of A_N, where $A_N = D^{-½} A D^{-½}$.
- Draw a random Gaussian (normal) matrix Ω
- Form $Y = A_N{}^{q}\,\Omega$
- Compute skinny QR: $QR = Y$

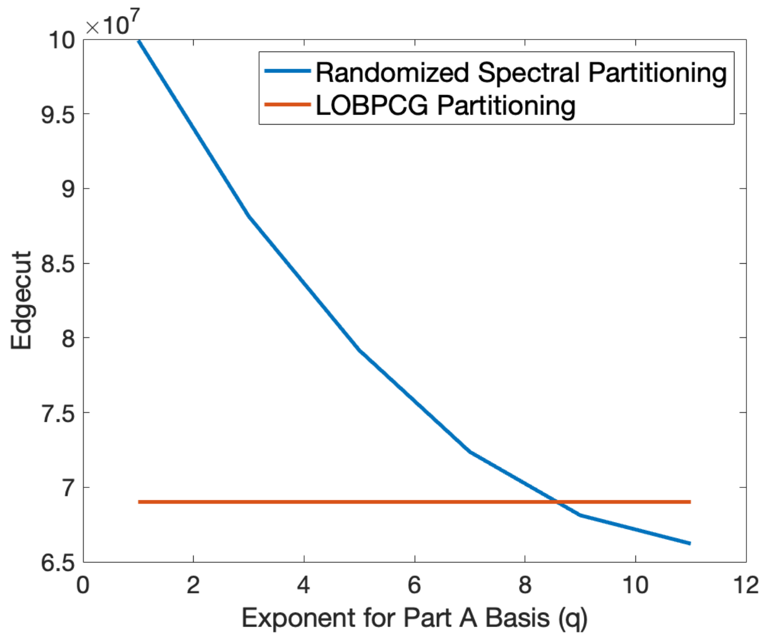
Randomized Method: Phase 2

- Second, compute eigenvalues on the projected problem.
- Compute projection $B = Q^TAQ$
- Solve eigenproblem for B: $B = V \lambda V^T$
- Project back: $U= QV$

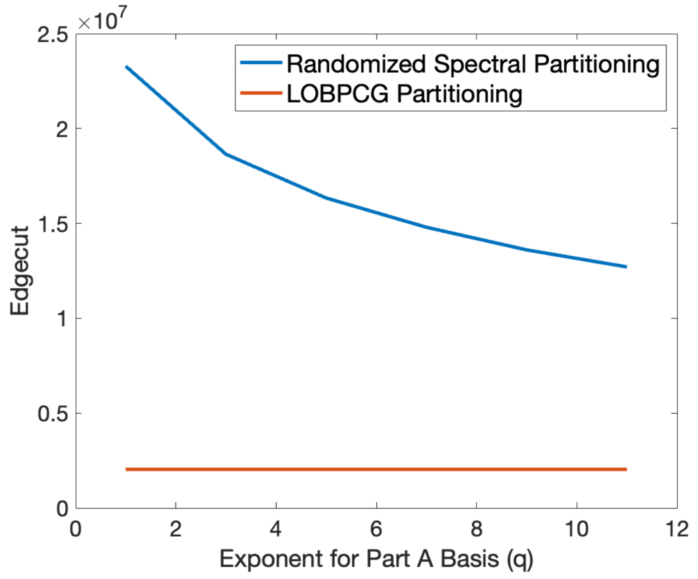
- We only need to solve a small, dense eigenproblem for B
  - Fast!
  - No longer need LOBPCG (or any sparse eigensolver)

Randomized partitioning quality

Irregular: Hollywood



Regular: Brick3d



The randomized eigensolver actually works *better* than LOBPCG for partitioning with sufficiently large q (for irregular graphs)!

Results: Quality

Sphynx edge cuts with LOBPCG vs randomized solver with L=20.

Matrix	LOBPCG	q=1	q=3	q=5	q=7	q=9	q=11
cube100	2,036,942	23,280,878	18,643,406	16,339,232	14,763,242	13,620,082	12,645,466
hollywood	69,010,728	99,913,222	88,136,872	79,170,890	72,369,774	68,120,278	66,220,826
wikipedia	70,372,336	82,607,424	80,328,958	77,783,740	74,965,720	71,660,478	69,205,042
FullChip	19,837,100	21,925,964	18,723,240	17,296,392	16,483,600	15,890,706	15,466,674
Circuit5M	40,918,466	52,793,074	49,117,806	42,290,548	33,731,544	31,757,878	31,563,734

Randomized method (q=11) often gives lower (better) cuts than LOBPCG !

Results: Run Time

Sphynx run times (CPU) with LOBPCG vs randomized solver with L=20.

Matrix	LOBPCG	q=1	q=3	q=5	q=7	q=9	q=11
cube100	18.19	1.601	2.185	2.779	3.357	3.907	4.465
hollywood	360.6	5.865	10.88	15.69	20.44	25.33	30.35
wikipedia	923.3	18.59	33.28	47.75	62.15	76.45	90.84
FullChip	162.8	5.00	6.24	7.50	8.79	10.13	11.38
Circuit5M	821.5	11.14	13.98	16.23	18.27	21.04	23.93

Our randomized method is 10X-80X faster (q=1) than LOBPCG!
Also much faster with q=11.

Conclusions

- Randomized eigensolver can dramatically speed up (5-80X) a spectral partitioner
- Works well for irregular graphs (e.g., web graphs) but not so well for more regular graphs (e.g., meshes)
- Trade-off in computational cost vs quality
- Sphynx has been released in Trilinos/Zoltan2
  - Randomized method will be released soon
- All spectral methods have some weaknesses
  - Can benefit from multilevel methods and edge-cut refinement
  - Collaboration with K. Madduri and M. Gilbert (Penn State) will address this
- Approach can be extended to spectral clustering
  - Is randomized linear algebra useful in other discrete problems?

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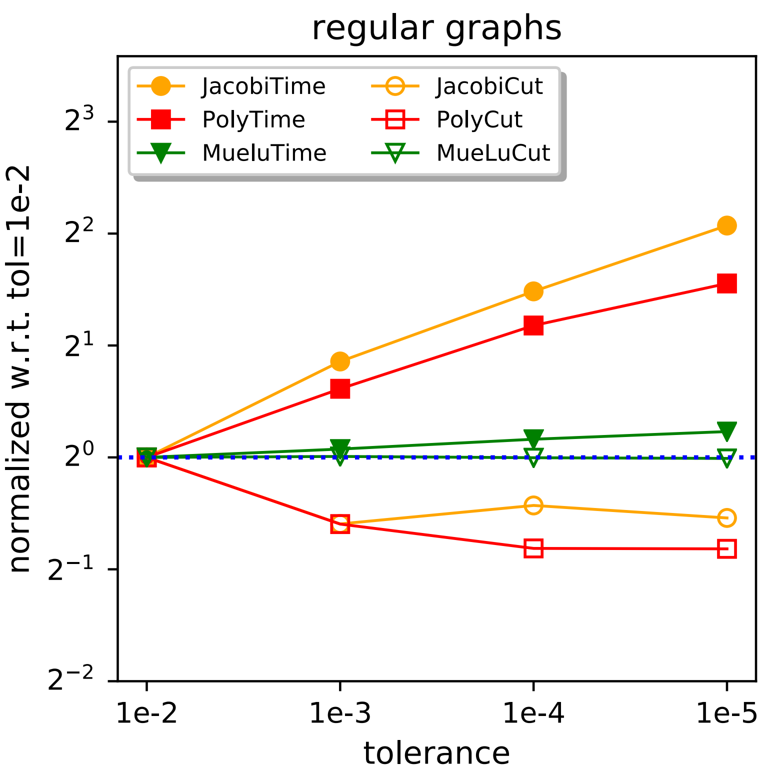
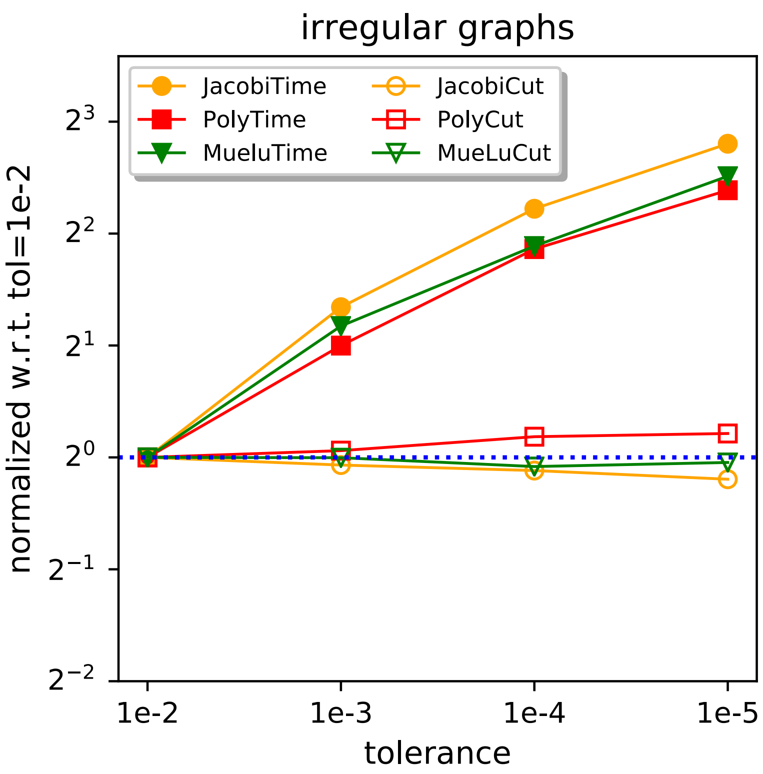
Extra slides

Sphynx – Results

LOBPCG Convergence Tolerance:





<u>Default:</u> 1e-2 for MueLu

1e-3 for others

<u>Default:</u> 1e-2 for all

Sphynx – Results

Eigenvalue Problem:

Average results normalized w.r.t combinatorial					
		generalized		normalized	
	preconditioner	runtime	cutsize	runtime	cutsize
regular	Jacobi	0.81	1.15	0.43	2.26
	Polynomial	0.73	1.21	0.54	2.45
	MueLu	0.99	1.12	0.95	2.20
irregular	Jacobi	0.75	0.83	0.26	1.36
	Polynomial	0.36	0.84	0.02	0.83
	MueLu	0.71	0.90	0.31	1.68

Default: combinatorial for regular graphs,

generalized for irregular graphs with Jacobi and MueLu, and

normalized for irregular graphs with Polynomial.

Sphynx – Results

Preconditioner:

Average results normalized w.r.t. Jacobi				
	Polynomial		**MueLu**	
	runtime	cutsize	runtime	cutsize
regular	0.46	1.03	**0.42**	**0.91**
irregular	**0.62**	**1.71**	1.91	0.94

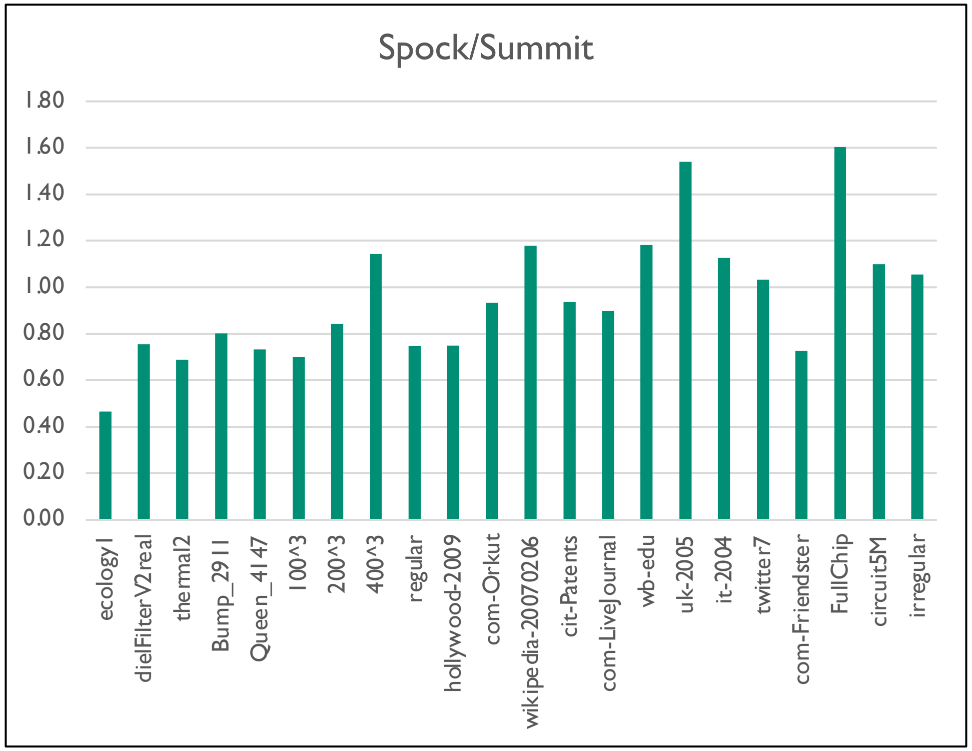
Suggested: MueLu for regular graphs,

Polynomial for irregular graphs.

Sphynx: Exascale Systems

Sphynx Running Time on OLCF systems:

- Summit: Nvidia Volta V100
- Spock: AMD MI200



RUNNING TIME (s)			
	Summit	Spock	Spock/Summit
ecology1	1.40	0.65	0.47
dielFilterV2real	2.13	1.61	0.75
thermal2	1.78	1.22	0.69
Bump_2911	1.68	1.35	0.80
Queen_4147	2.20	1.61	0.73
100^3	1.39	0.97	0.70
200^3	2.11	1.78	0.84
400^3	6.78	7.75	1.14
geomean			**0.75**
hollywood-2009	4.79	3.60	0.75
com-Orkut	8.06	7.52	0.93
wikipedia-20070206	15.66	18.44	1.18
cit-Patents	8.27	7.75	0.94
com-LiveJournal	8.70	7.81	0.90
wb-edu	5.54	6.55	1.18
uk-2005	89.31	137.59	1.54
it-2004	90.24	101.58	1.13
twitter7	482.85	499.43	1.03
com-Friendster	186.16	135.20	0.73
FullChip	48.36	77.56	1.60
circuit5M	43.55	47.87	1.10
geomean			**1.05**