Detecting Anomalies in Very Large Graphs

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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Example Applications of Graph Analytics

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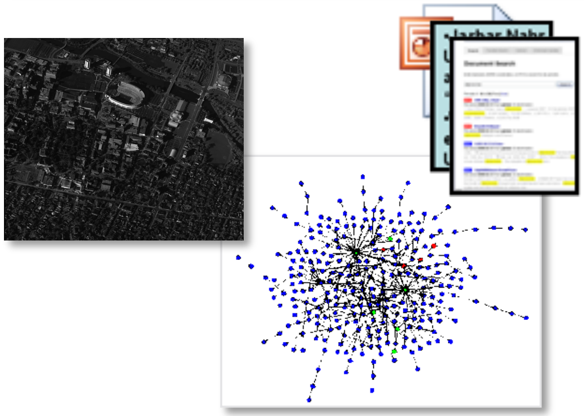
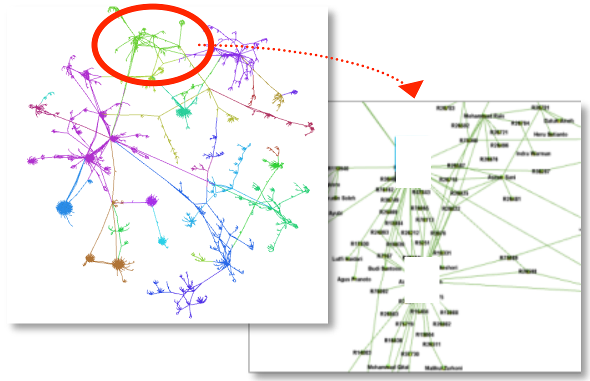
ISR	Social	Cyber

ISR



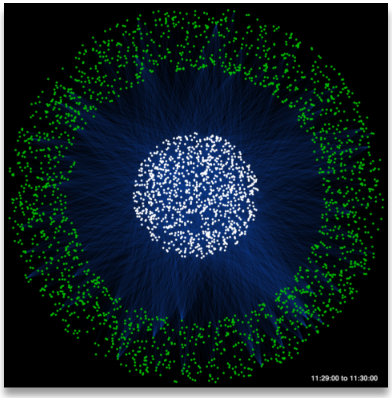
- Graphs represent entities and relationships detected through multiple sources
- 1,000s – 1,000,000s tracks and locations
- GOAL: Identify anomalous patterns of life

Social



- Graphs represent relationships between individuals or documents
- 10,000s – 10,000,000s individual and interactions
- GOAL: Identify hidden social networks

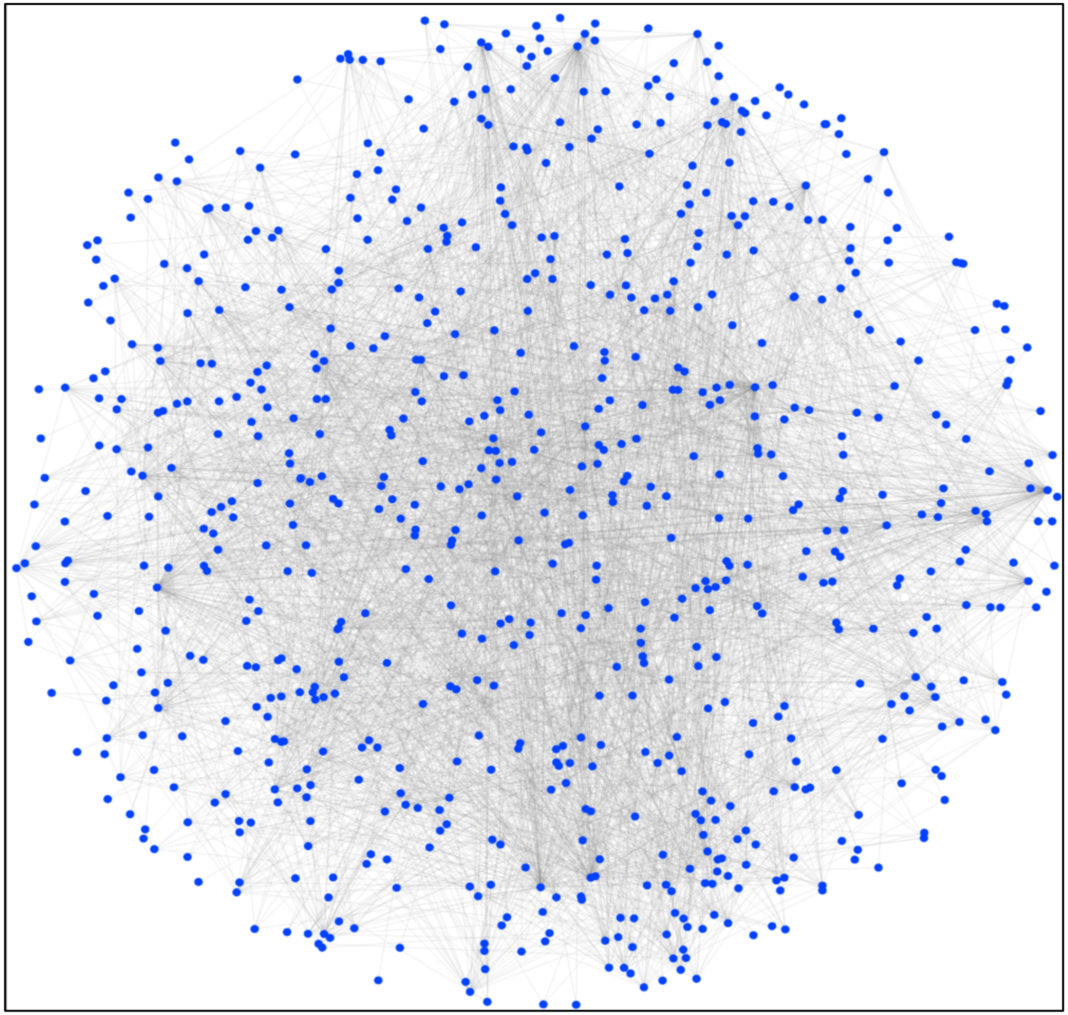
Cyber



- Graphs represent communication patterns of computers on a network
- 1,000,000s – 1,000,000,000s network events
- GOAL: Detect cyber attacks or malicious software

Cross-Mission Challenge:
Detection of subtle patterns in massive multi-source noisy datasets

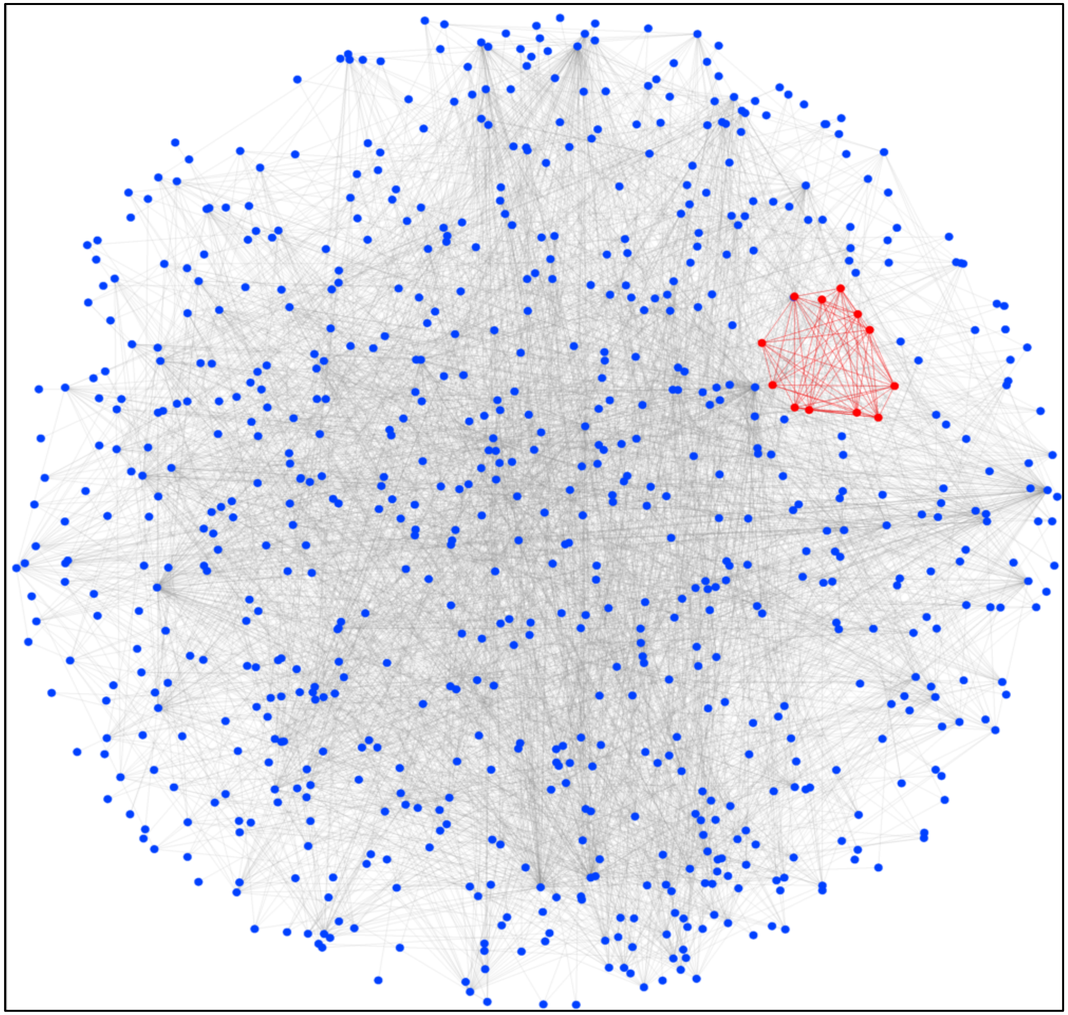
Example: Network Traffic Surrogate



Graph Statistics

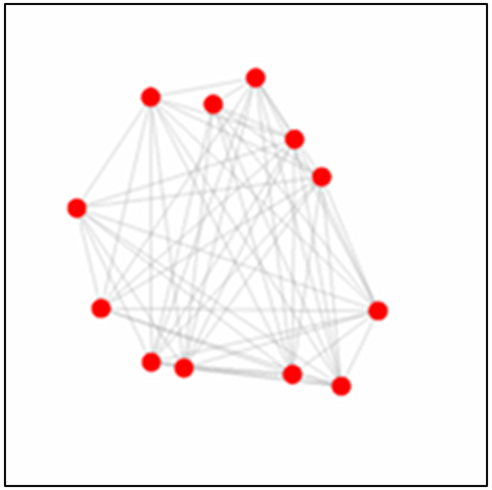
- **R-Mat**
- **Parameters derived from network traffic data**
- **1024 vertices**

Big Data Challenge: Activity Signatures



Graph Statistics

- **R-Mat**
- **Parameters derived from network traffic data**
- **1024 vertices**
- **Anomaly: 12 vertices**
- **Anomaly: 1% of graph (often smaller)**

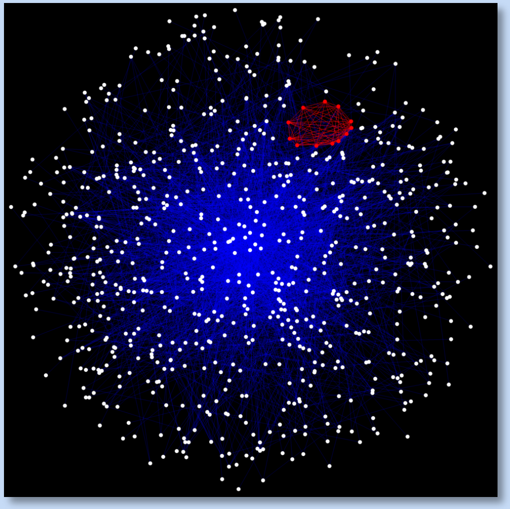


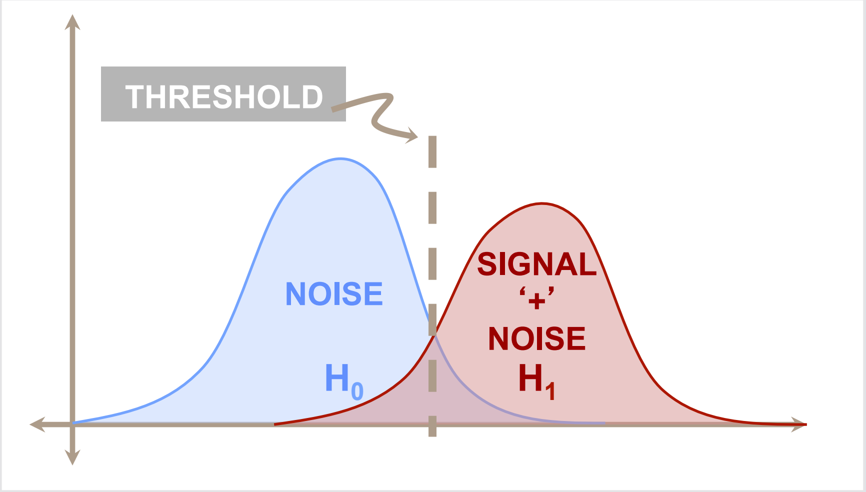
Challenge: Activity signature is typically a weak signal

Outline

- Anomaly Detection in Very Large Graphs
- ➡ Signal Processing for Graphs (SPG)
- Improving Sparse Matrix-Vector Multiplication (SpMV) Performance through 2D Partitioning
- Partitioning: Dynamic Graphs and Sampling
- Summary

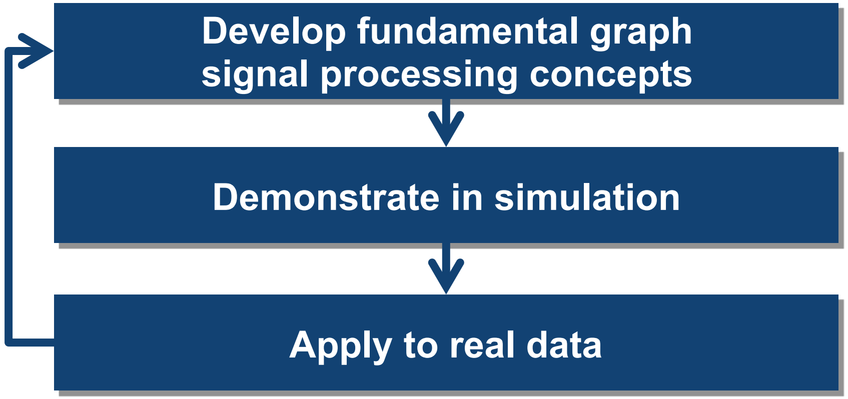
Statistical Detection Framework for Graphs



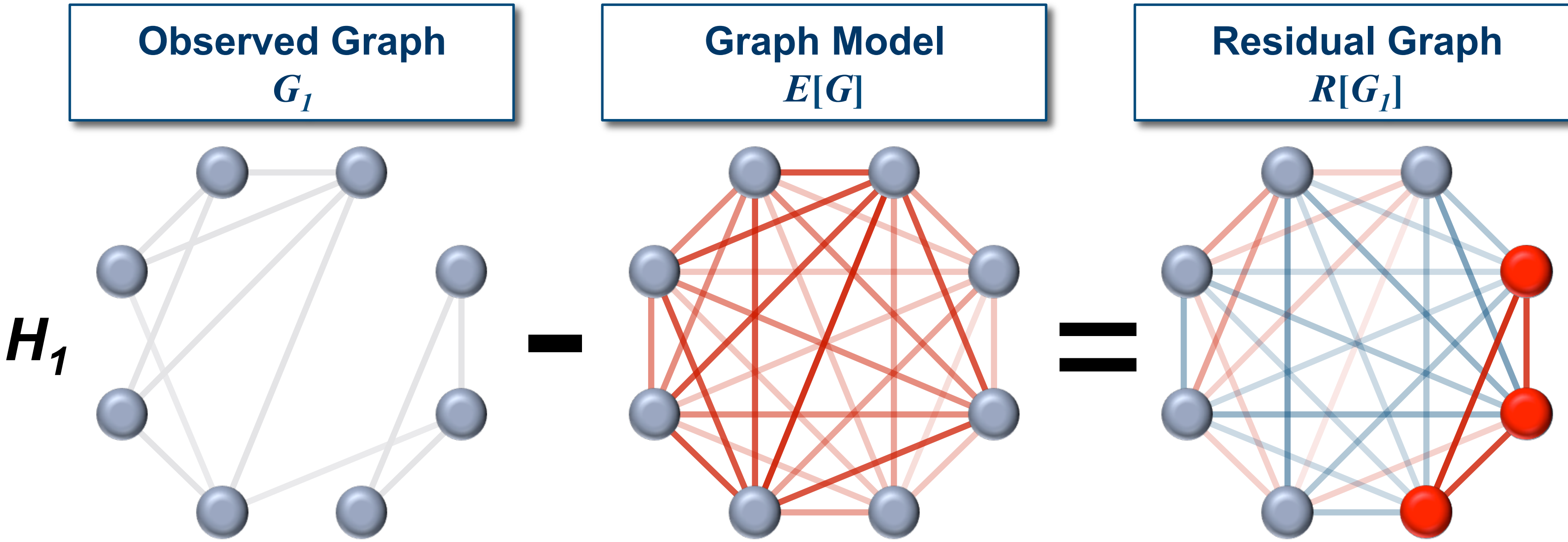


Graph Theory

Detection Theory



Residuals Example: Anomalous Subgraph



- Residual graph represents the difference between the observed and expected
- *Coordinated* vertices (subsets of vertices connected by edges with large edge weights) in residual graph will produce much stronger signal than uncoordinated vertices

Detection framework is designed to detect coordinated deviations from the expected topology

SPG Processing Chain

DIMENSIONALITY REDUCTION

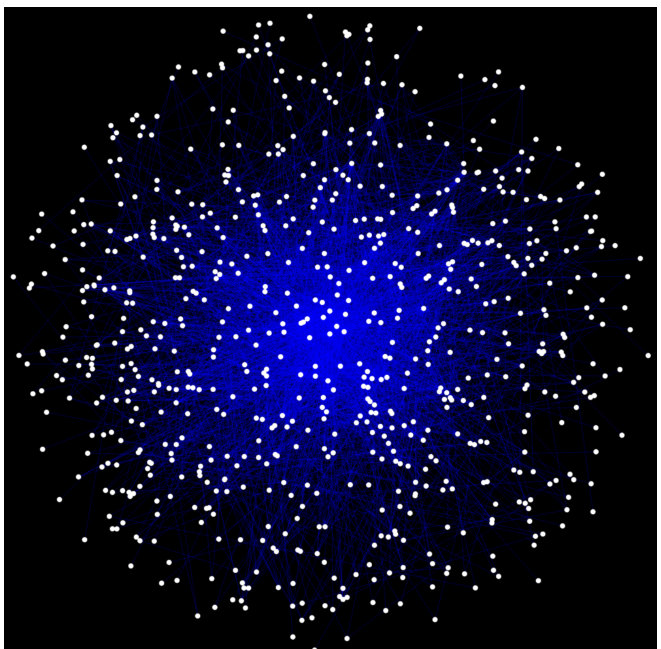
Temporal Integration → Graph Model Construction → Residual Decomposition → Component Selection → Anomaly Detection → Identification

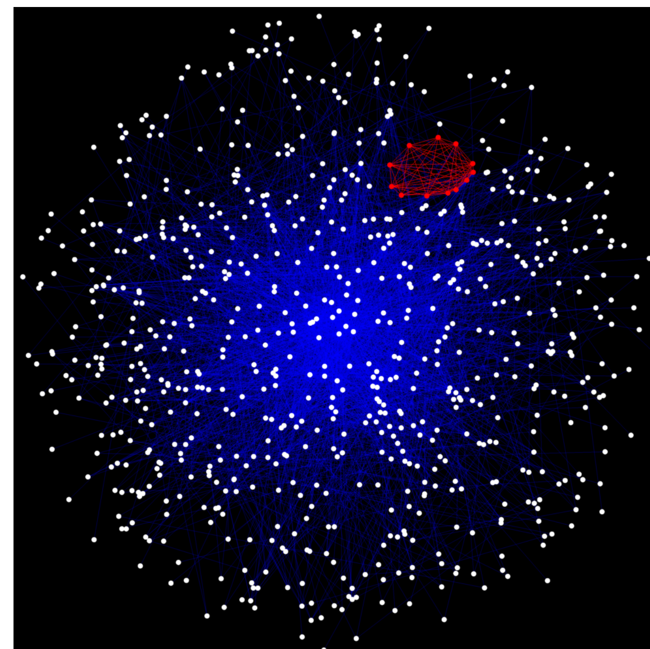
Input

- Graph
- No cue

Output

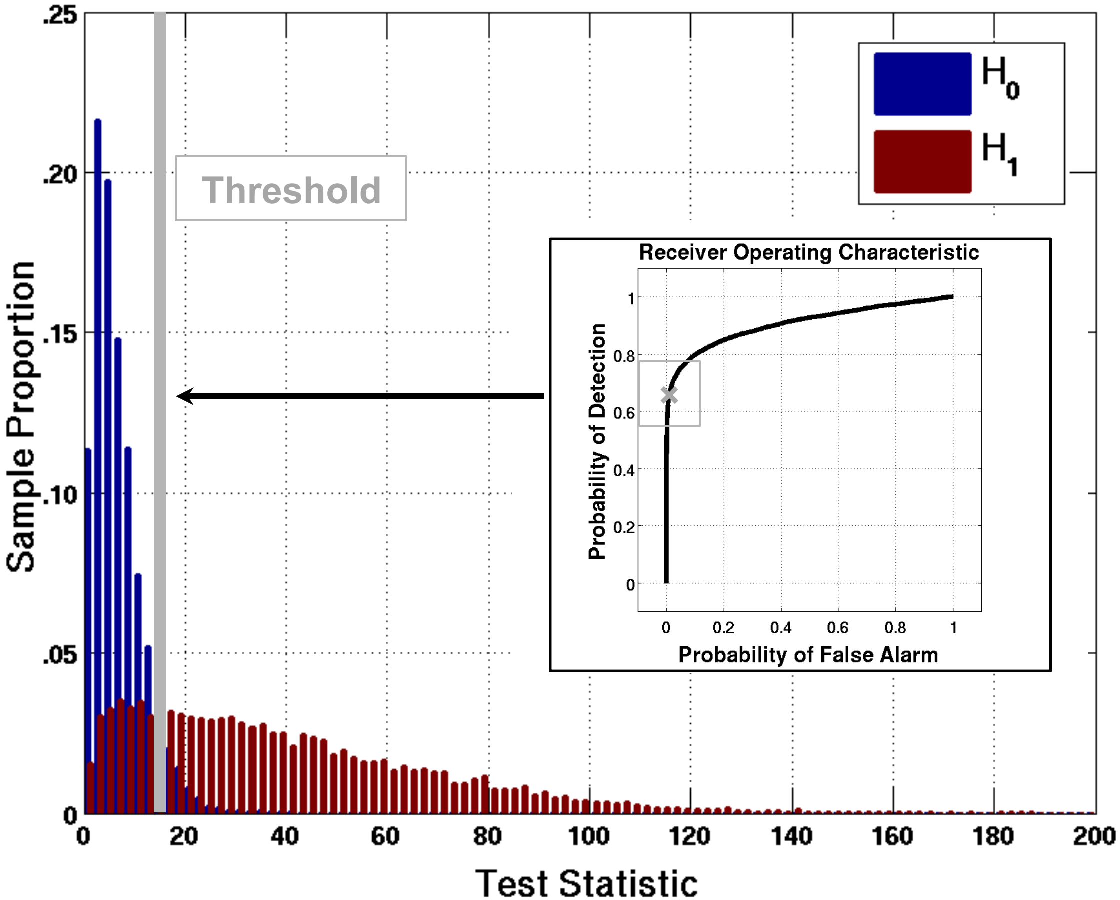
- Statistically anomalous subgraph(s)





Anomaly Detection: Setup Phase

TEMPORAL INTEGRATION → GRAPH MODEL CONSTRUCTION → RESIDUAL DECOMPOSITION → COMPONENT SELECTION → **ANOMALY DETECTION** → IDENTIFICATION



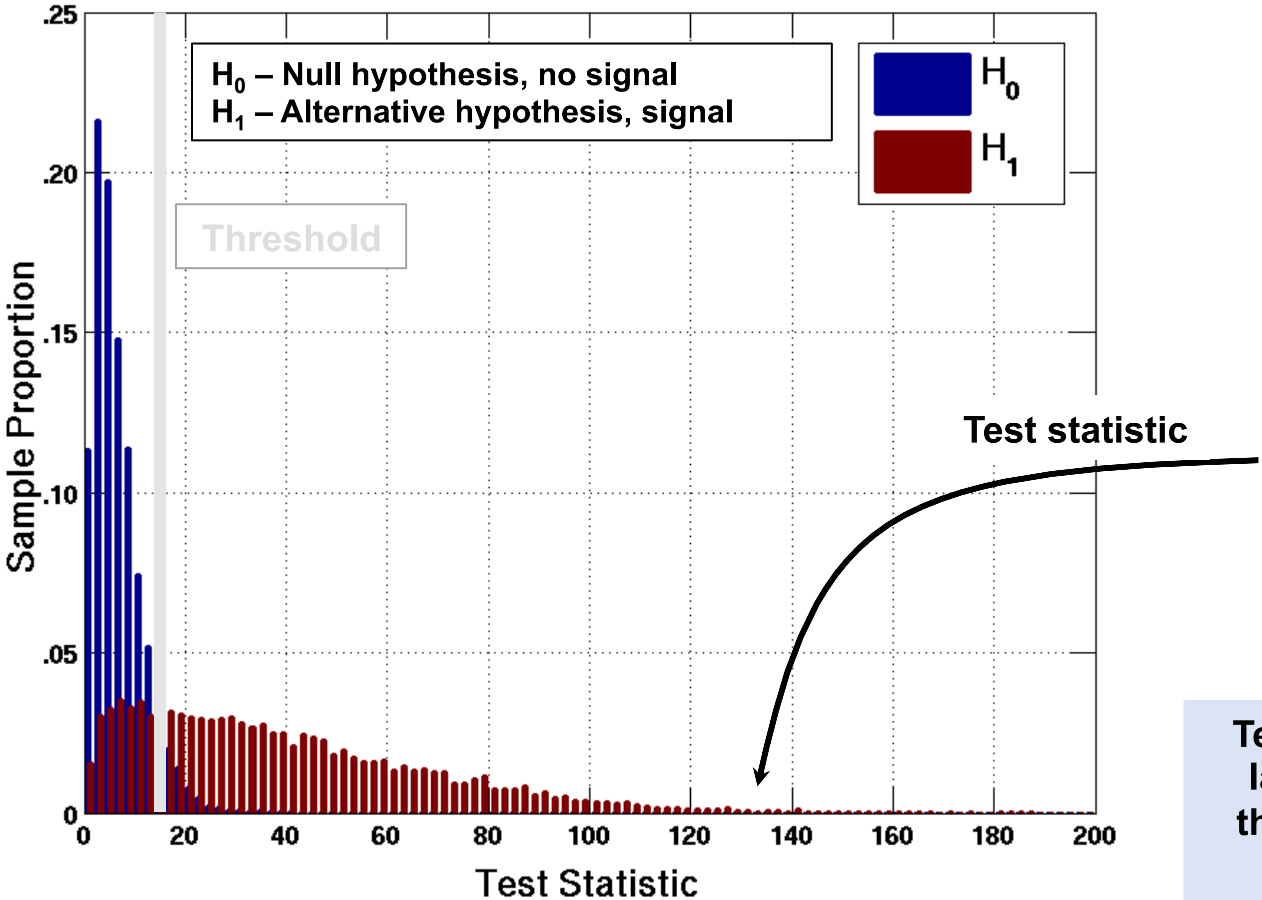
H_0 – Null hypothesis, no signal
H_1 – Alternative hypothesis, signal

Detection Setup

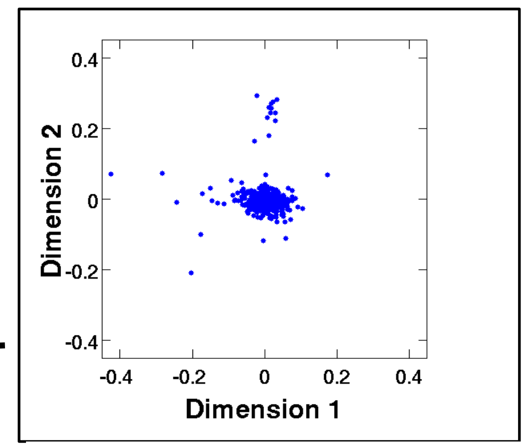
1. Monte-Carlo simulations to generate density functions
2. ROC-curve generated from density function

Anomaly Detection

Temporal Integration → Graph Model Construction → Residual Decomposition → Component Selection → **Anomaly Detection** → Identification



Test statistic calculated for observed graph:



$$\chi^2_{\max} = \max_{\theta} \chi^2 \left(\begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} [u_1 \; u_2]^T \right)$$

Test statistic value significantly larger than test statistic value threshold corresponding to 1% false alarm rate

Computational Focus: Dimensionality Reduction

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DIMENSIONALITY REDUCTION

TEMPORAL INTEGRATION → GRAPH MODEL CONSTRUCTION → RESIDUAL DECOMPOSITION → COMPONENT SELECTION → ANOMALY DETECTION → IDENTIFICATION

Eigensystem

$$B = (A - E[A])$$

Solve:

$$Bx_i = \lambda_i x_i, i = 1, \ldots, m$$

Example: Modularity Matrix

$$E[A_s] = k\, k^T / (2|e|)$$

$|e|$ – Number of edges in graph $G(A)$

k – degree vector

k_i = degree(v_i), $v_i \in G(A)$

- Dimensionality reduction dominates computation
- Eigen decomposition is key computational kernel
- Parallel implementation required for very large graph problems
  - Fit into memory, minimize runtime

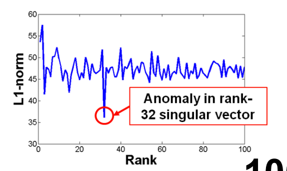
Need fast parallel eigensolvers

Detection Methods, Effectiveness, and Cost

Notional Comparison of Power and Effectiveness

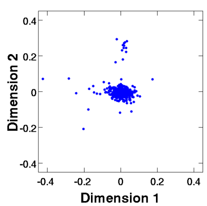
Detection Power

Eigenvectors L_1 Norms



100s EVs

χ^2 in 2 Principal Components



2 EV

Spectral Norm

σ_1, λ_1

1 EV

Computation Cost

- **More powerful methods require more computation**
- **For detection of subtle anomalies, need to calculate 100s of eigenvectors fast**

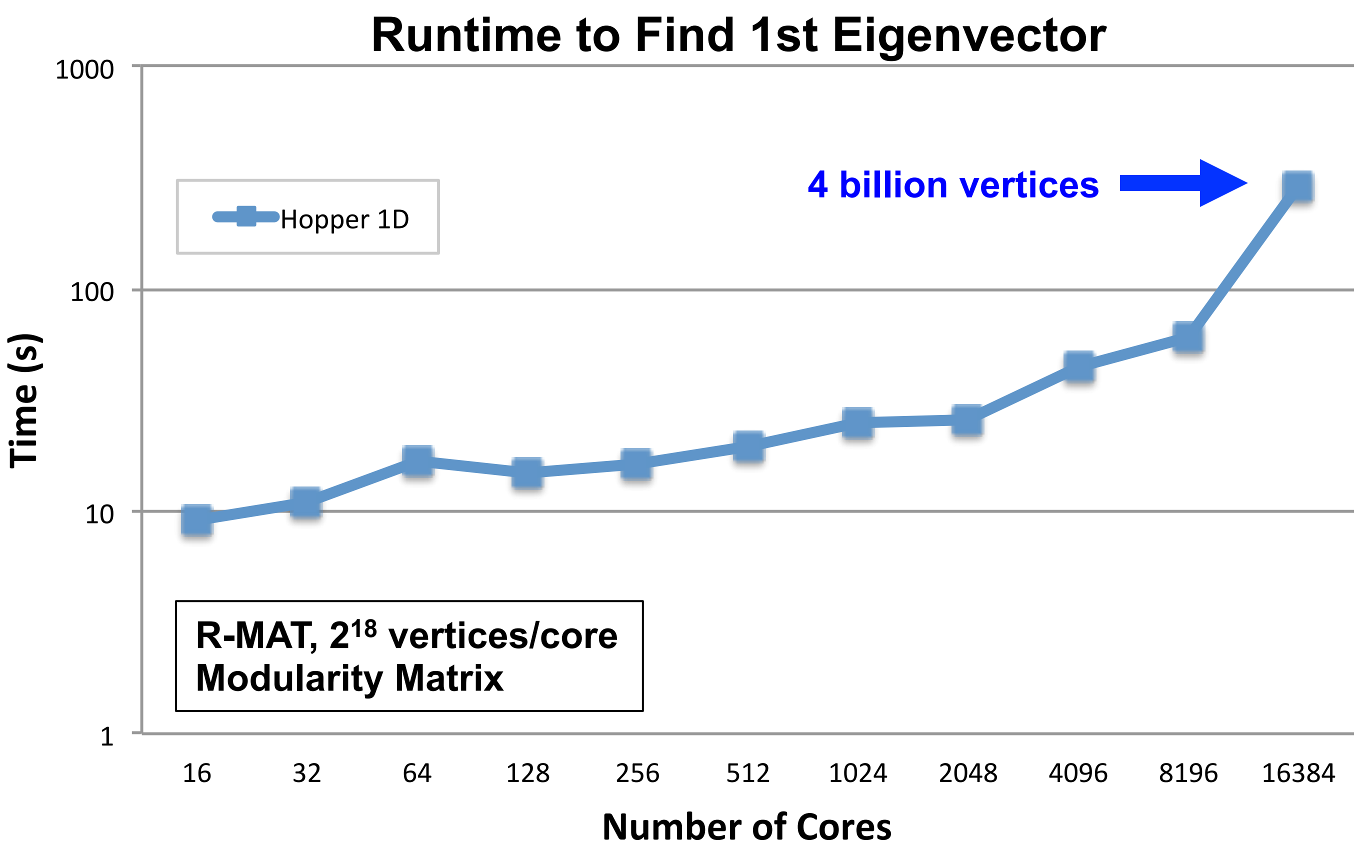
$O((|E|r+|V|r^2+r^3)h)^*$ **to compute r eigenvectors**

Parallel Implementation

- Using Anasazi (Trilinos) Eigensolver
  - Block Krylov-Schur
  - Eigenpairs corresponding to eigenvalues with largest real component
  - User defined operators (don’t form matrix explicitly)

- Initial Numerical Experiments
  - R-Mat (a=0.5, b=0.125, c=0.125, d=0.25)
    - Average nonzeros per row: 8
    - Number of rows: 2^{22} to 2^{32}
  - Two systems
    - LLGrid (MIT LL) – compute cluster (10 GB ethernet)
    - Hopper* (NERSC) -- Cray XE6 supercomputer
  - Initially: 1D random row distribution (good load balance)

Weak Scaling – Hopper*

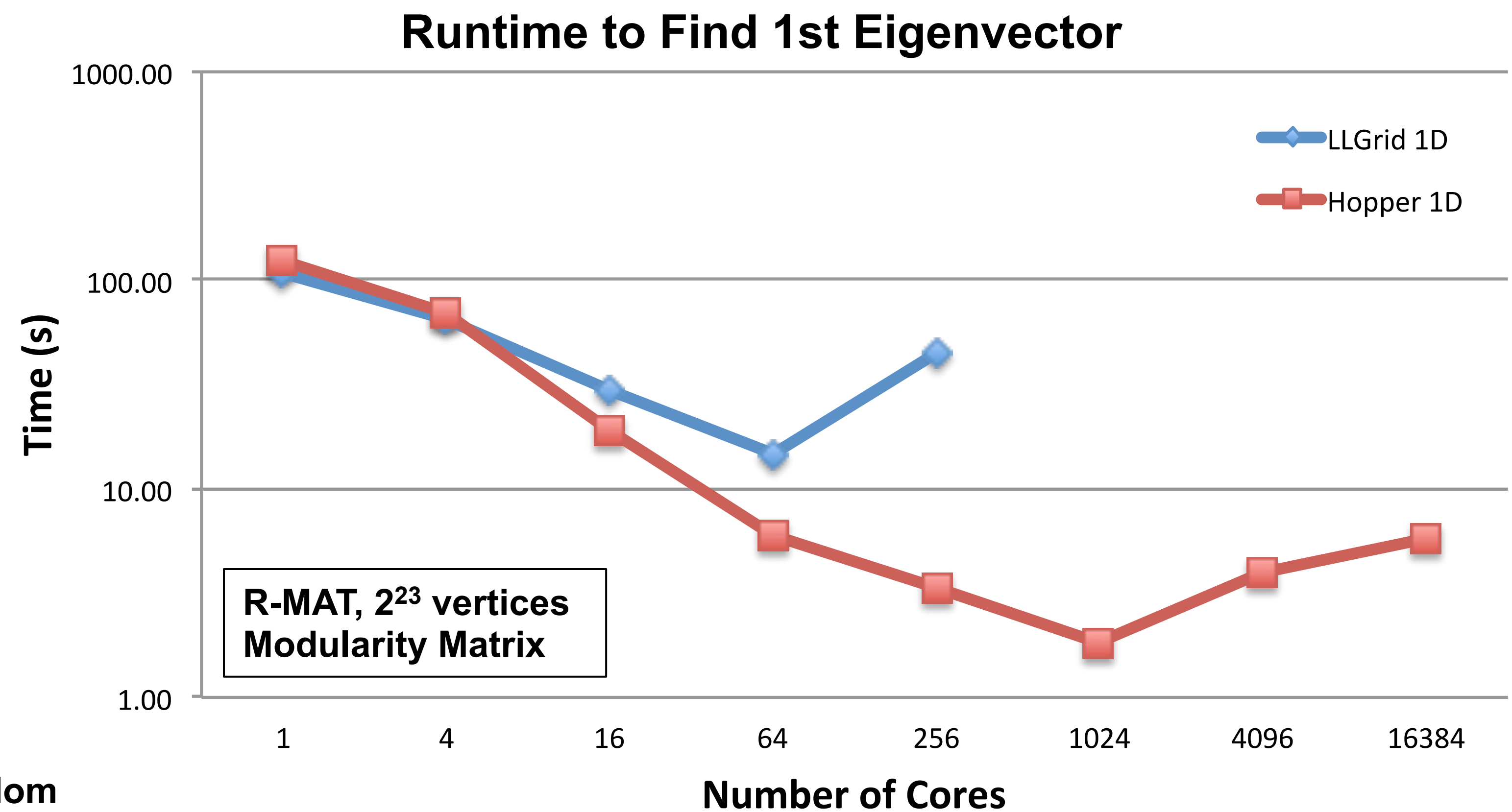


1D random partitioning

Solved system for up to 4 billion vertex graph

* This research used resources of the National Energy Research Scientific Computing Center, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

Strong Scaling Results



1D random partitioning

Scalability limited and runtime increases for large numbers of cores

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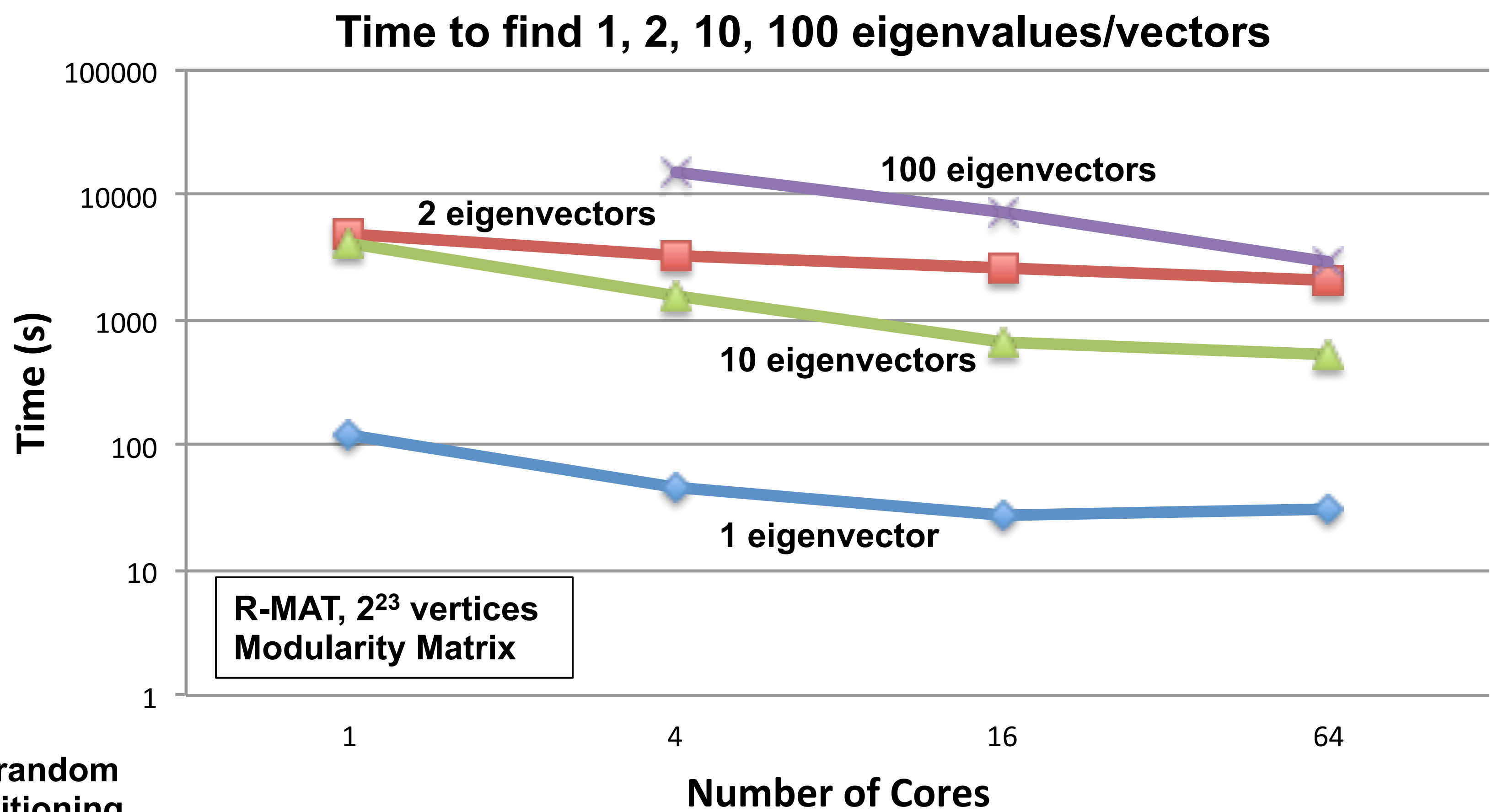
Finding Multiple Eigenvectors – LLGrid



1D random partitioning

LLGrid system

Significant increase in runtime when finding additional eigenvectors

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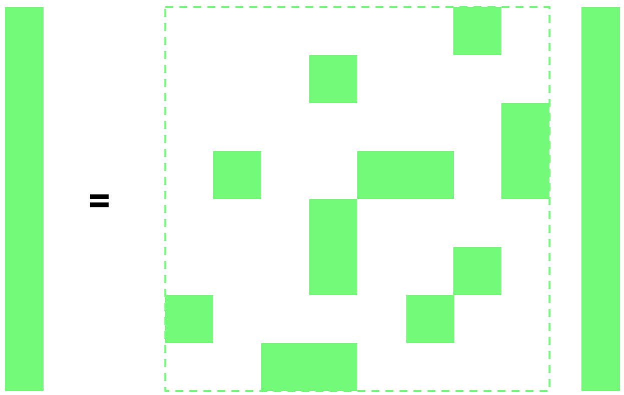
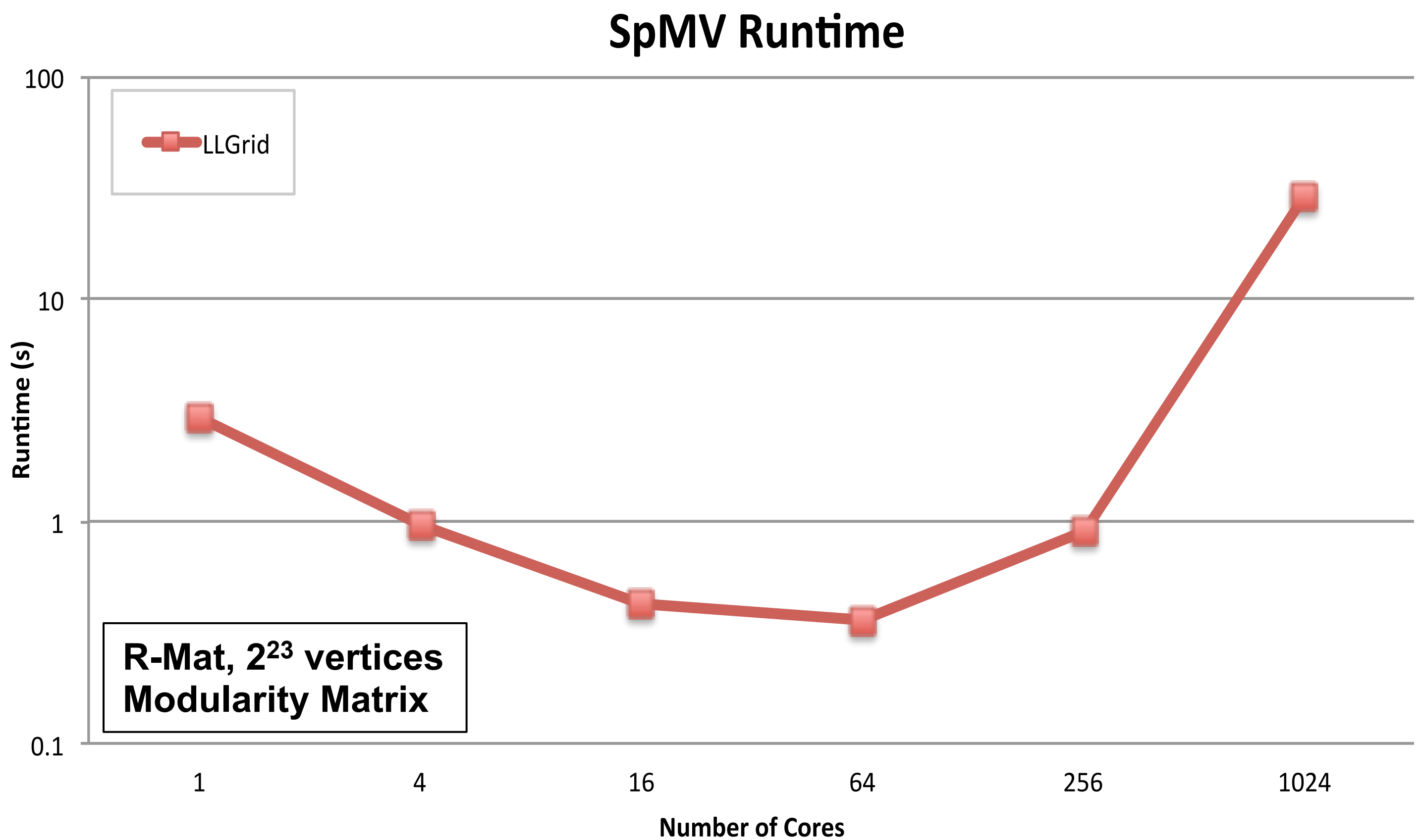
Sparse Matrix-Vector Multiplication



- Sparse matrix-dense vector multiplication (SpMV) key computational kernel in eigensolver
- Performance of SpMV challenging for matrices resulting from power-law graphs
  - Load imbalance
  - Irregular communication
  - Little data locality
- Important to improve performance of SpMV

SpMV Strong Scaling -- LLGrid



1D random partitioning

Scalability limited and runtime increases for large numbers of cores

Data Partitioning to Improve SpMV

$$
\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ y_6 \\ y_7 \\ y_8 \end{bmatrix} = \begin{bmatrix} 1 & 6 & 0 & 0 & 0 & 0 & 0 & 0 \\ 5 & 1 & 9 & 0 & 5 & 0 & 0 & 0 \\ 0 & 8 & 1 & 7 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 1 & 0 & 0 & 0 & 7 \\ 0 & 0 & 0 & 0 & 1 & 8 & 0 & 0 \\ 4 & 0 & 0 & 0 & 3 & 1 & 3 & 0 \\ 0 & 0 & 0 & 6 & 0 & 9 & 1 & 4 \\ 0 & 0 & 0 & 0 & 0 & 0 & 2 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \\ 4 \\ 3 \\ 1 \\ 4 \\ 2 \\ 1 \end{bmatrix}
$$

$$\mathbf{y} = \mathbf{A}\mathbf{x}$$

- Partition matrix nonzeros
- Partition vectors

Communication Pattern: 1D Block Partitioning

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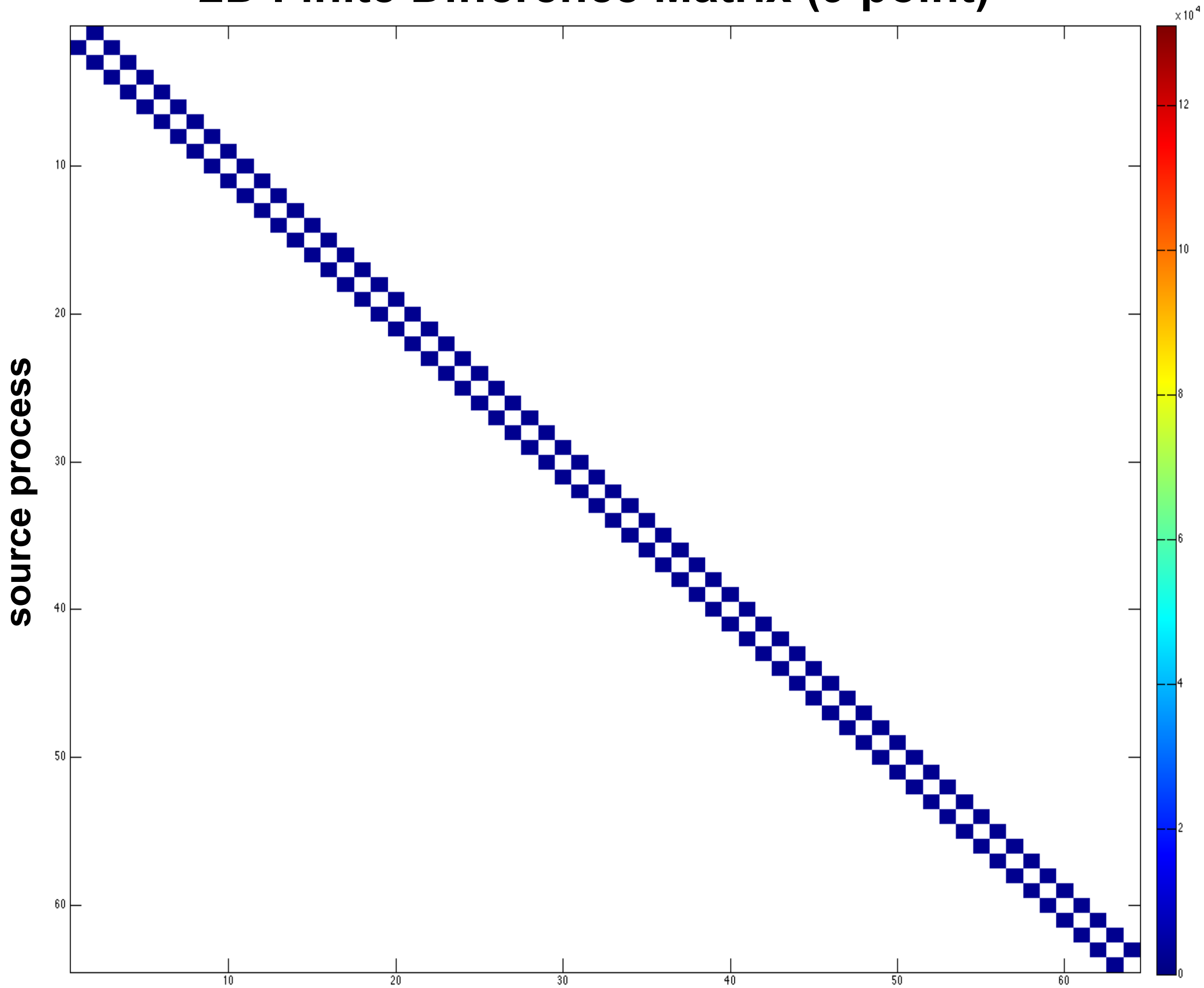
2D Finite Difference Matrix (9 point)



P=64

Number of Rows: 2^{23}
Nonzeros/Row: 9

NNZ/process

min: 1.17E+06
max: 1.18E+06
avg: 1.18E+06
max/avg: 1.00

 # Messages (Phase 1)

total: 126
max: 2

Volume (Phase 1)

total: 2.58E+05
max: 4.10E+03

Nice properties:

Great load balance
Small number of messages
Low communication volume

Communication Pattern: 1D Random Partitioning

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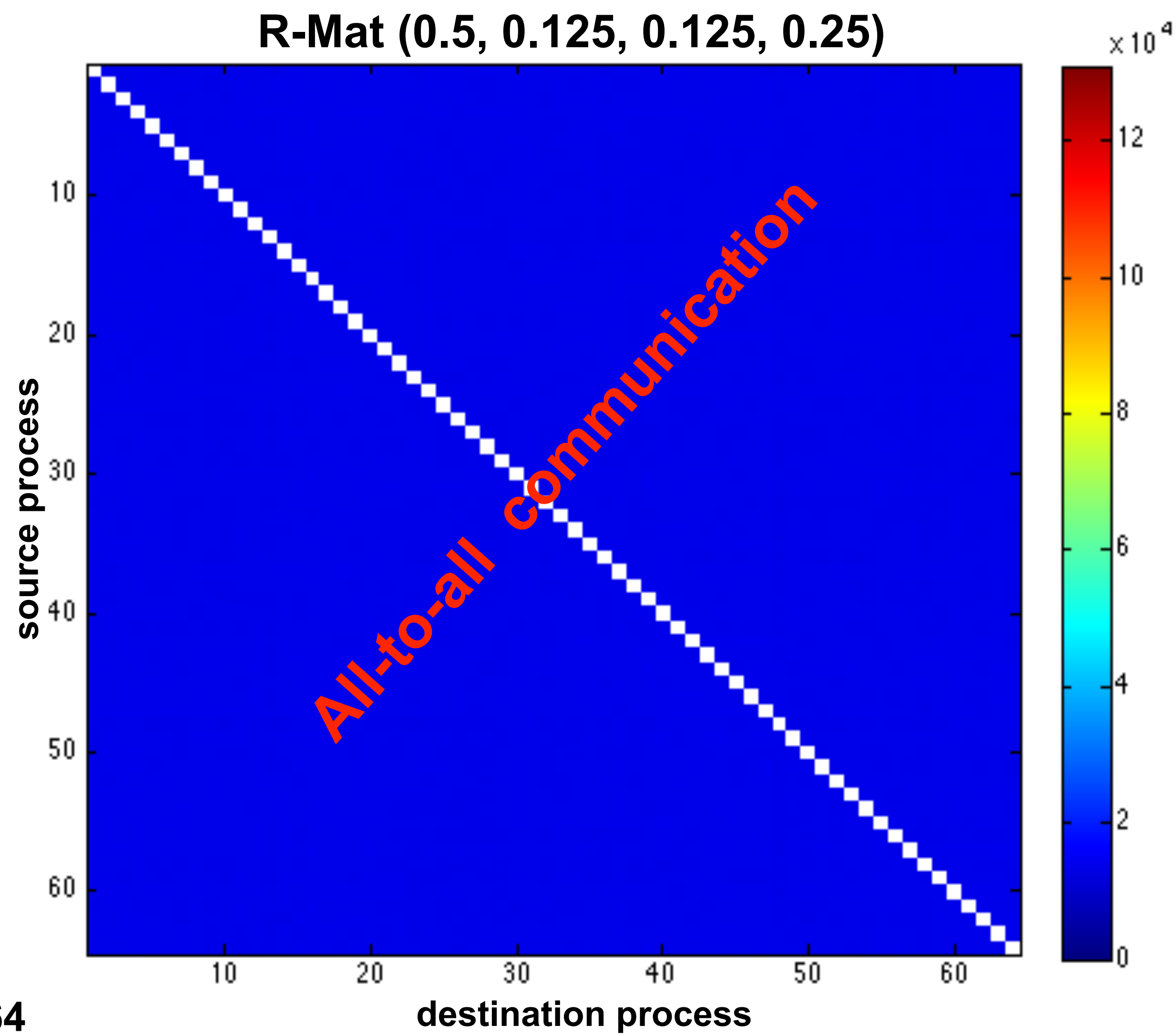


P=64

Number of Rows: 2^{23}
Nonzeros/Row: 8

NNZ/process
min: 1.05E+06
max: 1.07E+06
avg: 1.06E+06
max/avg: 1.01

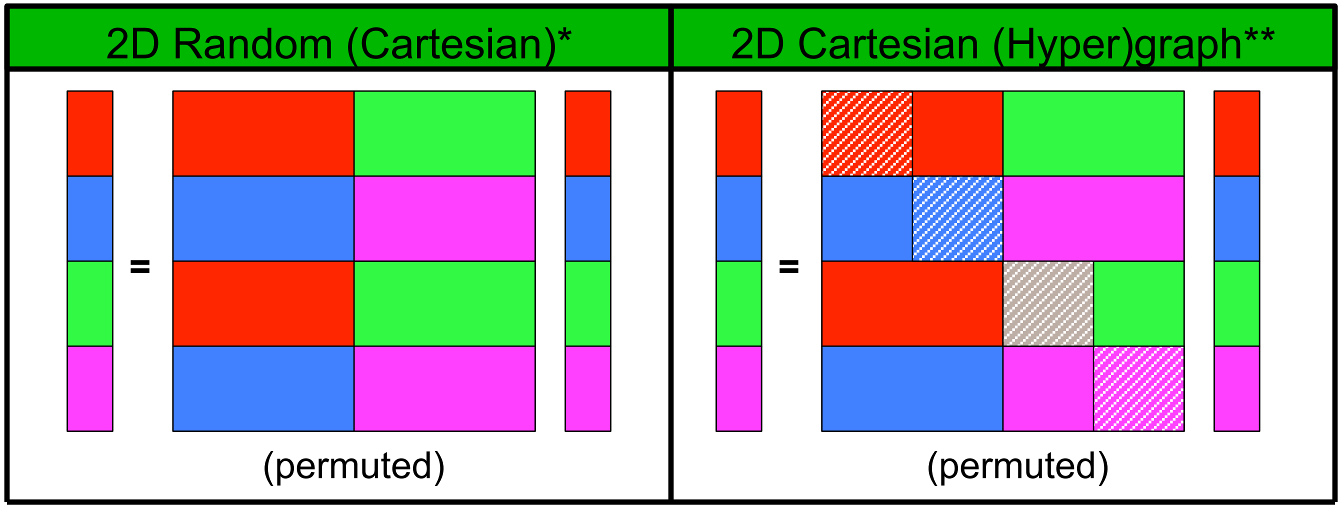
 # Messages (Phase 1)
total: 4032
max: 63

Volume (Phase 1)
total: 5.48E+07
max: 8.62E+05

Nice properties:
Great load balance

Challenges:
All-to-all communication

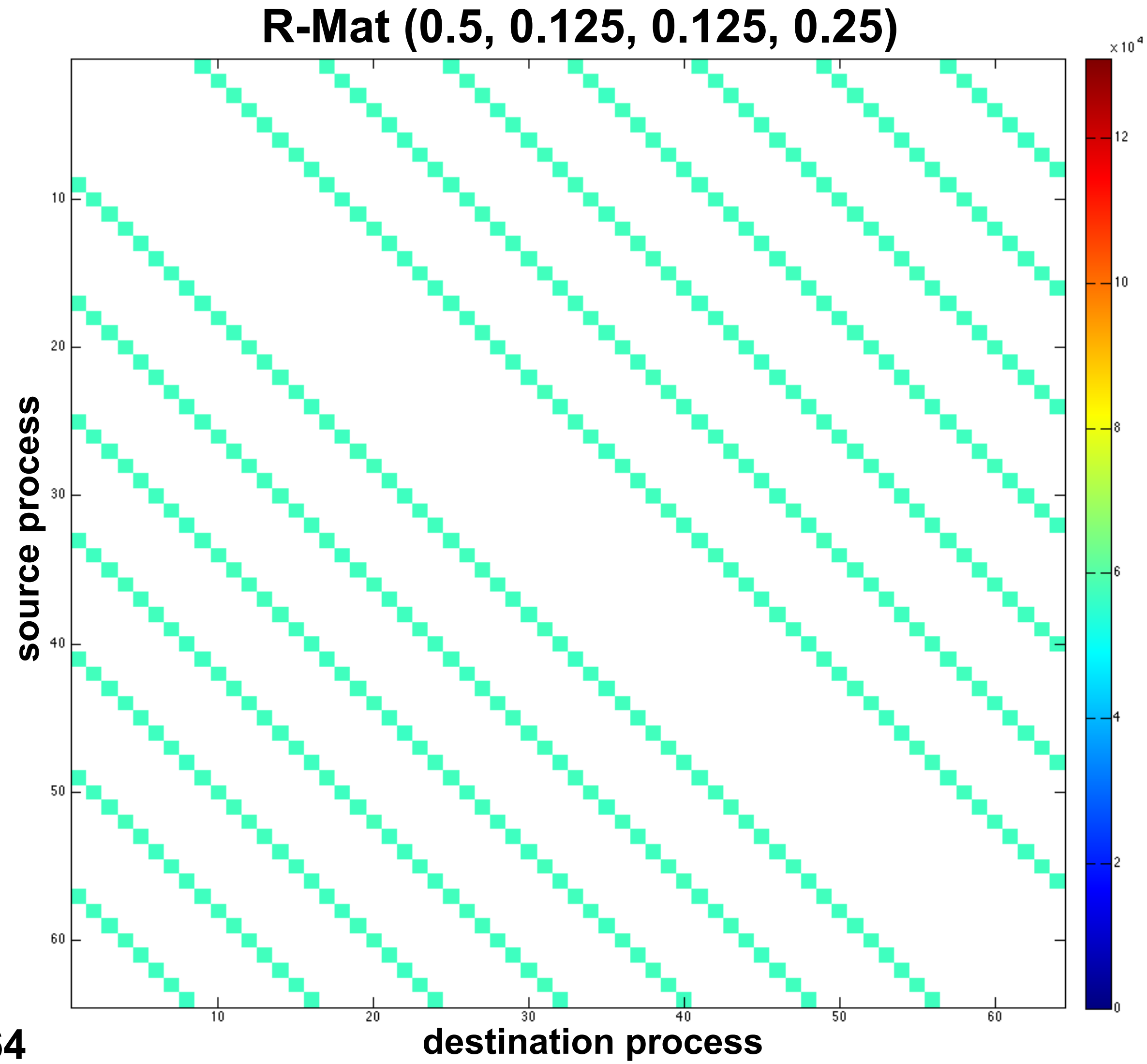
2D Partitioning



- 2D Partitioning
  - More flexibility: no particular part for entire row/column, more general sets of nonzeros
- Use flexibility of 2D partitioning to bound number of messages
  - Distribute nonzeros in permuted 2D Cartesian block manner
- 2D Random (Cartesian)*
  - Block Cartesian with rows/columns randomly distributed
  - Cyclic striping to minimize number of messages
- 2D Cartesian (Hyper)graph**
  - Replace random partitioning with hyper(graph) partititioning to minimize communication volume

*Hendrickson, et al.; Bisseling; Yoo, et al.
**Boman, Devine, Rajamanickam, “Scalable Matrix Computations on Large Scale-Free Graphs Using 2D Partitioning, SC2013.

Communication Pattern: 2D Random Partitioning Cartesian Blocks (2DR)



Number of Rows: 2^{23}
Nonzeros/Row: 8

NNZ/process
min: 1.04E+06
max: 1.05E+06
avg: 1.05E+06
max/avg: 1.01

 # Messages (Phase 1)
total: 448
max: 7

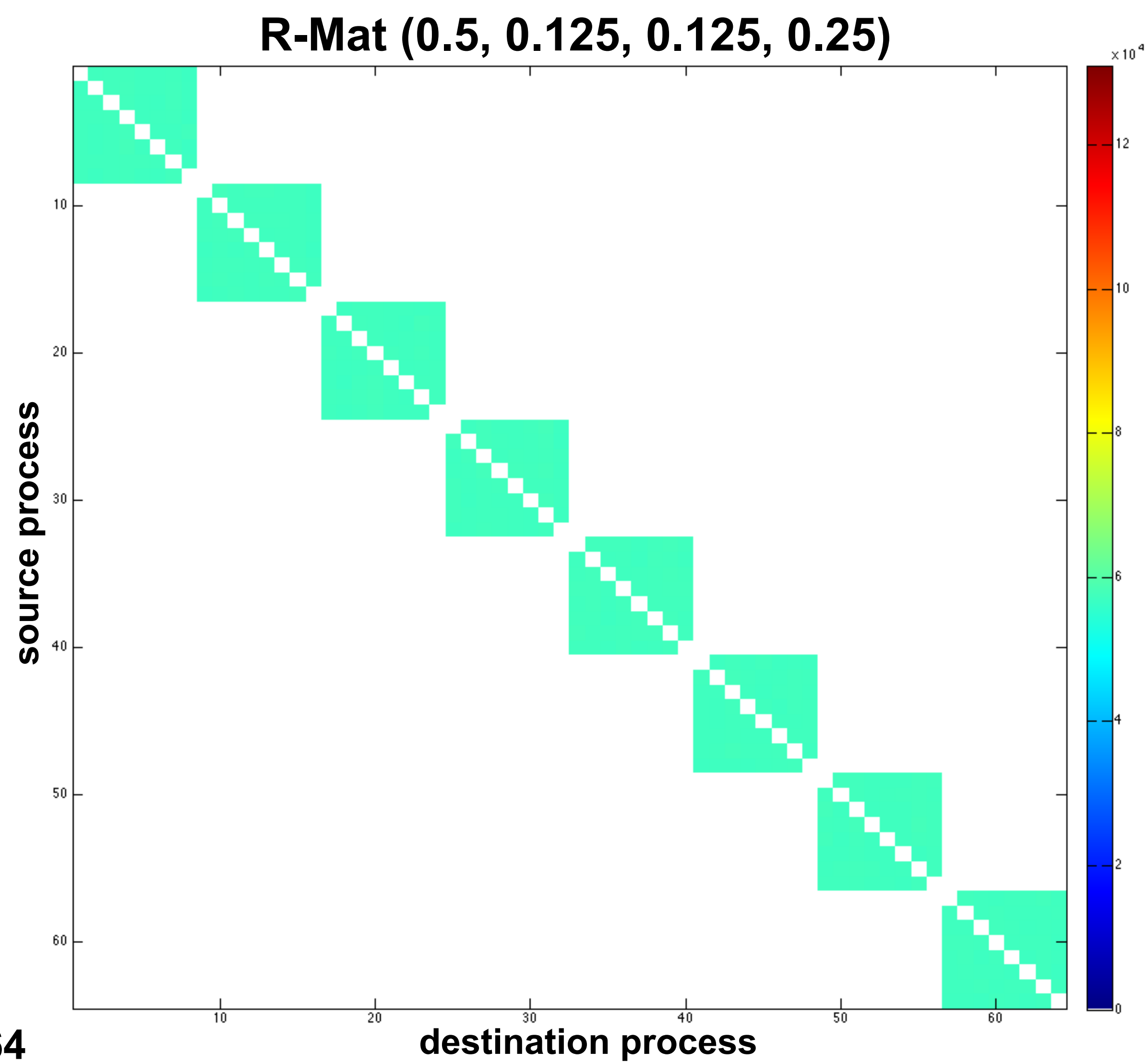
Volume (Phase 1)
total: 2.57E+07
max: 4.03E+05

Nice properties:
No all-to-all communication
Total volume lower than 1DR

P=64

1DR = 1D Random

Communication Pattern: 2D Random Partitioning Cartesian Blocks (2DR)



P=64

Number of Rows: 2^{23}
Nonzeros/Row: 8

NNZ/process
min: 1.04E+06
max: 1.05E+06
avg: 1.05E+06
max/avg: 1.01

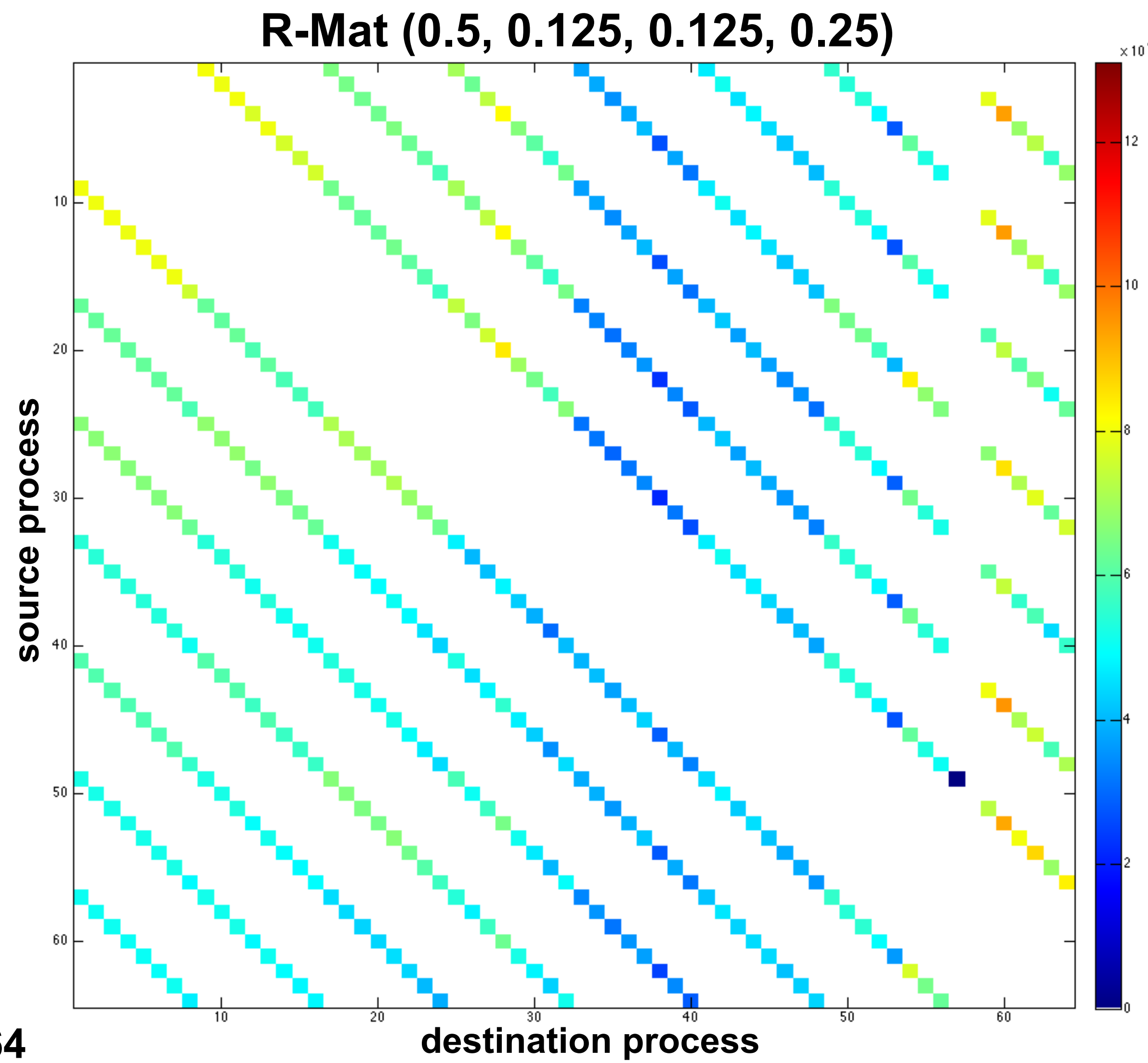
 # Messages (Phase 2)
total: 448
max: 7

Volume (Phase 2)
total: 2.57E+07
max: 4.03E+05

Nice properties:
No all-to-all communication
Total volume lower than 1DR

1DR = 1D Random

Communication Pattern: 2D Cartesian Hypergraph Partitioning



P=64

Number of Rows: 2^{23}
Nonzeros/Row: 8

NNZ/process
min: 5.88E+05
max: 1.29E+06
avg: 1.05E+06
max/avg: 1.23

 # Messages (Phase 1)
total: 448
max: 7

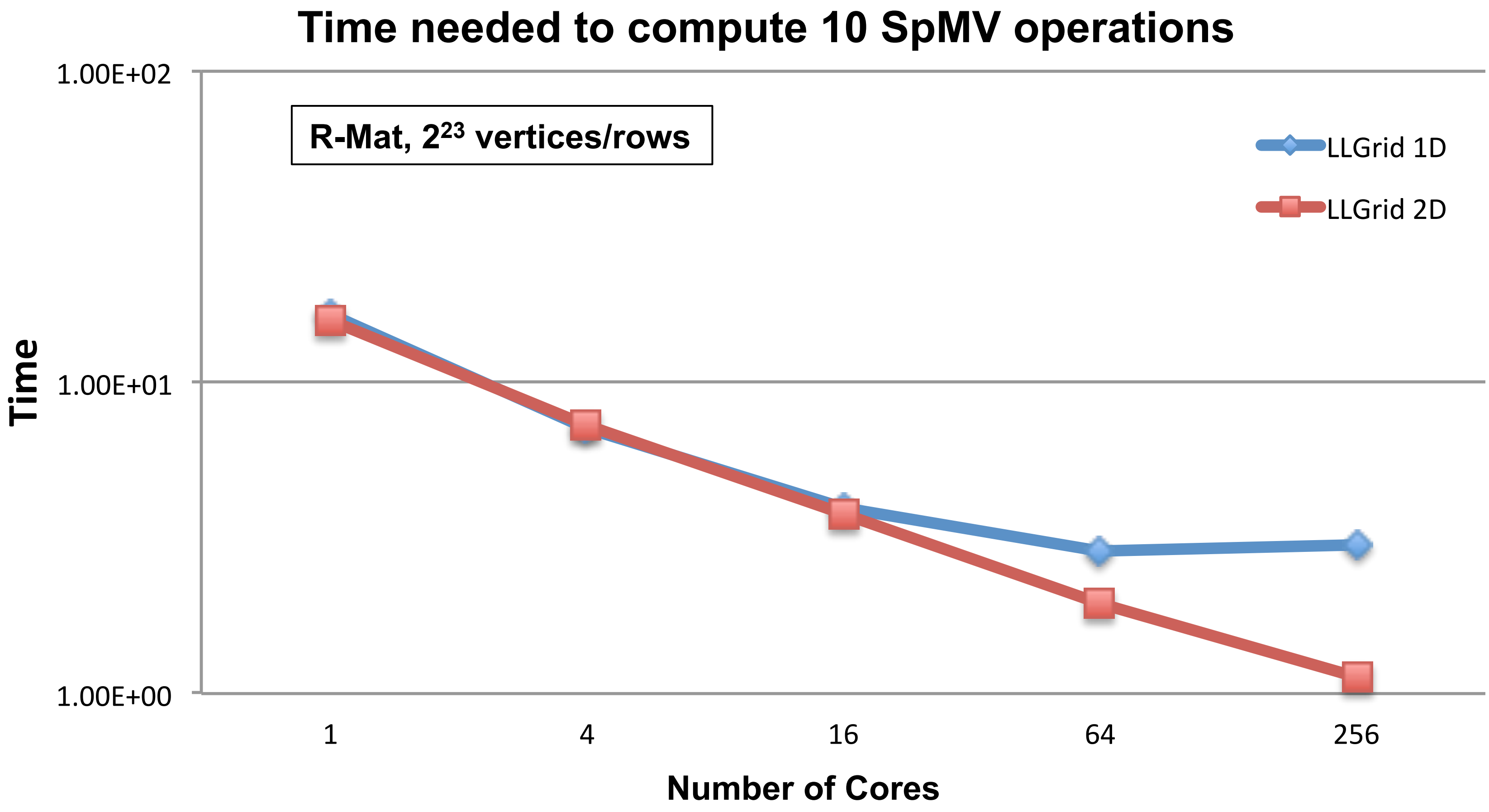
Volume (Phase 1)
total: 2.33E+07
max: 4.52E+05

Nice properties:
No all-to-all communication
Total volume lower than 2DR

Challenges:
Imbalance worse than 2DR

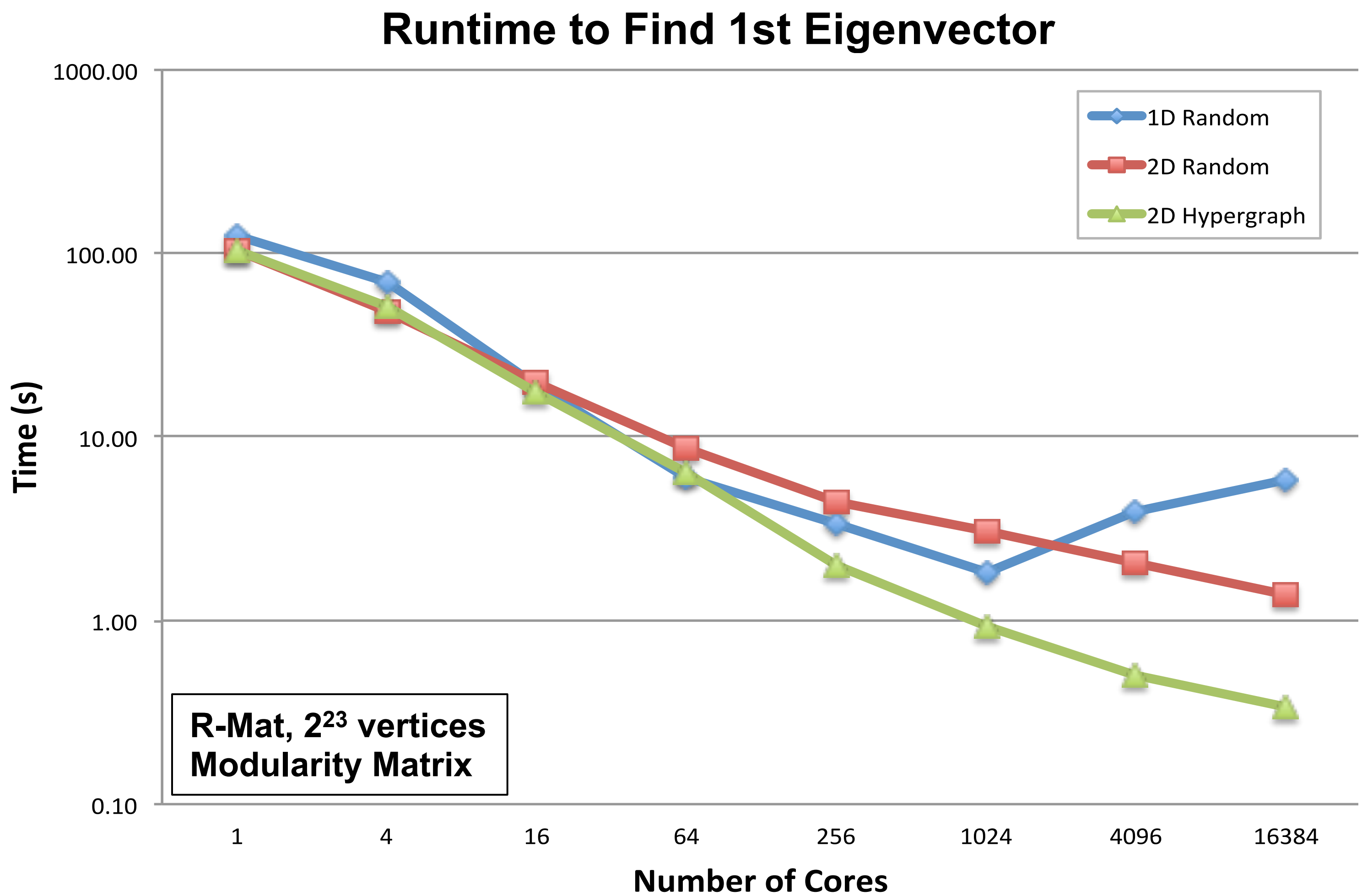
2DR = 2D Random Cartesian

Improved Results: SpMV – LLGrid



Simple 2D method shows improved scalability

Improved Results – NERSC Hopper*



2D methods show improved scalability

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Challenge with Hypergraph/Graph Partitioning

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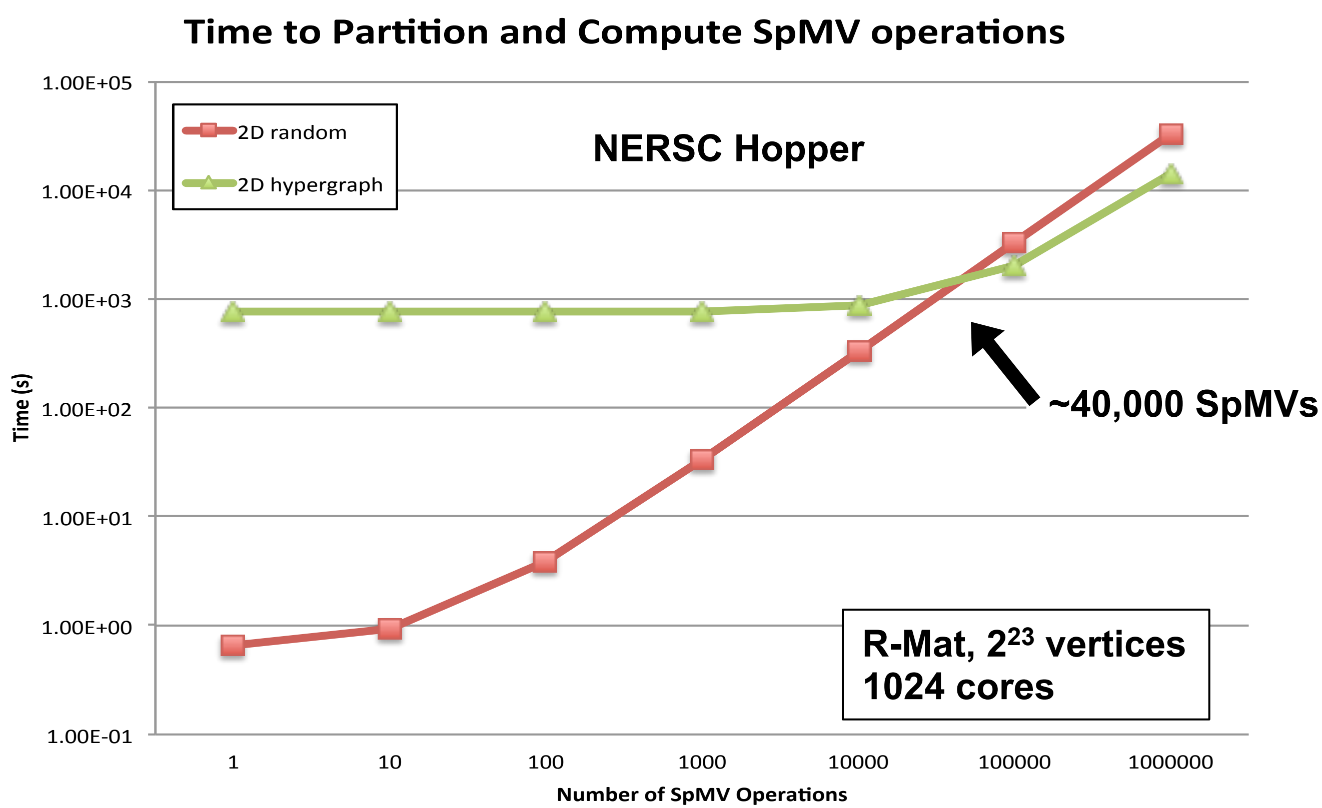
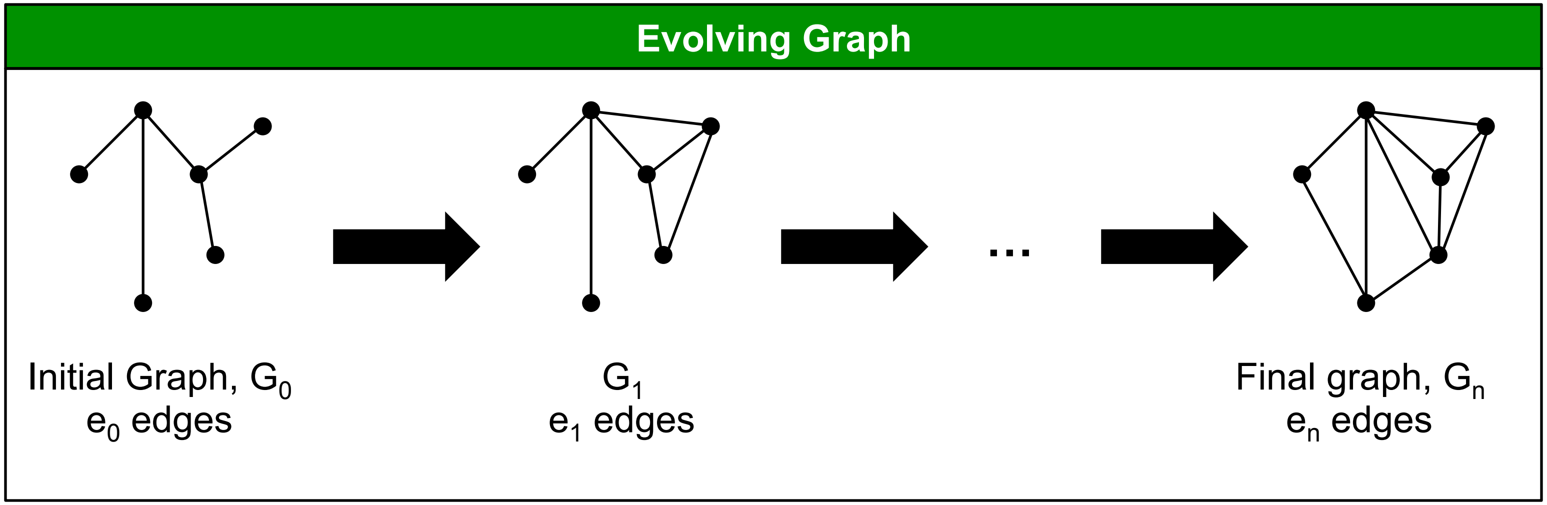


- High partitioning cost of graph/hypergraph methods must be amortized by computing many SpMV operations
- Detection* requires at most 1000s of SpMV operations
- Expensive partitions need to be effective for multiple graphs

*L1 norm method: computing 100 eigenvectors

Wolf, Miller: "Sparse Matrix Partitioning for Parallel Eigenanalysis of Large Static and Dynamic Graphs," *2014 IEEE HPEC Proc.*

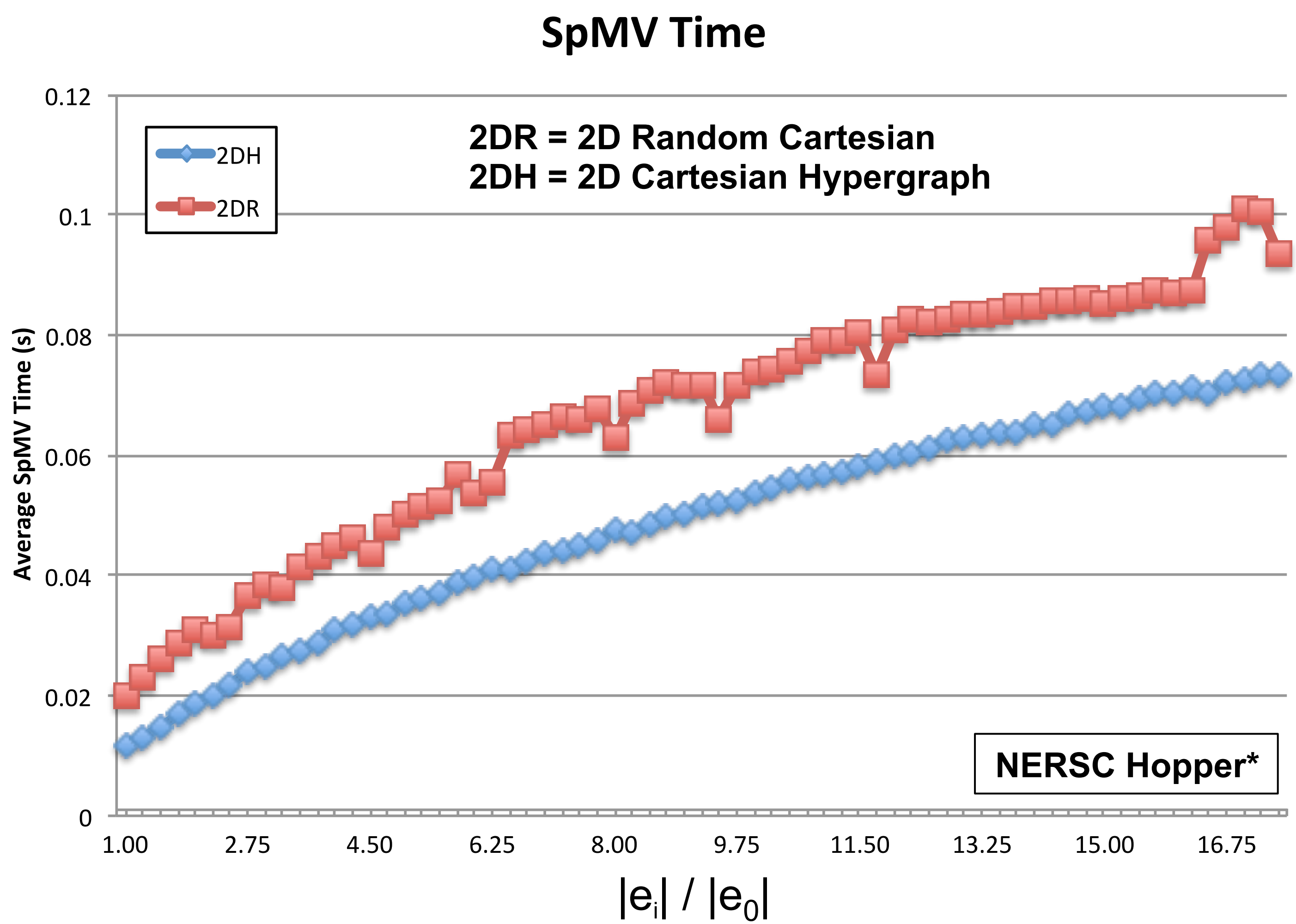
Experiment: Partitioning for Dynamic Graphs



- Key question: How long will a partition be effective?
- Initial experiment
  - Evolving R-Mat matrices: fixed number of rows, R-Mat parameters (a,b,c,d)
  - Start with a given number of nonzeros ($|e_0|$)
  - Iteratively add nonzeros until target number of nonzeros is reached ($|e_n|$)

Wolf, Miller: *2014 IEEE HPEC Proc.*

Results: Partitioning for Dynamic Graphs



Hypergraph partition surprising effective after more than 16x $|e_0|$ edges added

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Sampling and Partitioning for Web/SN Graphs

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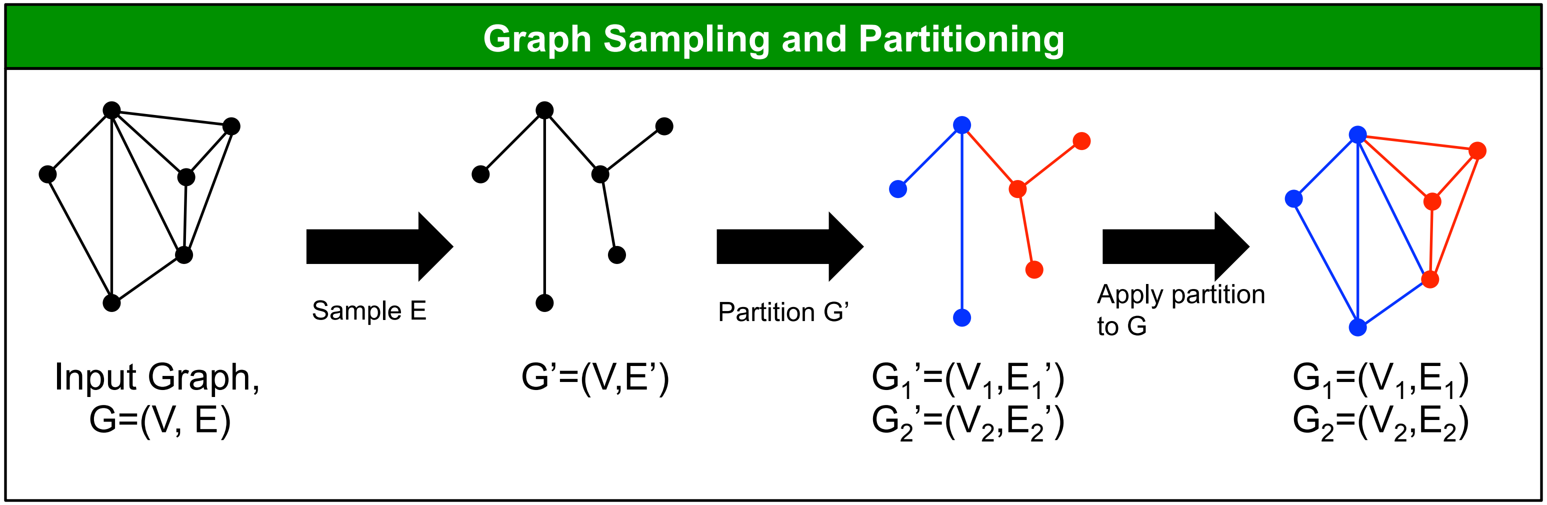
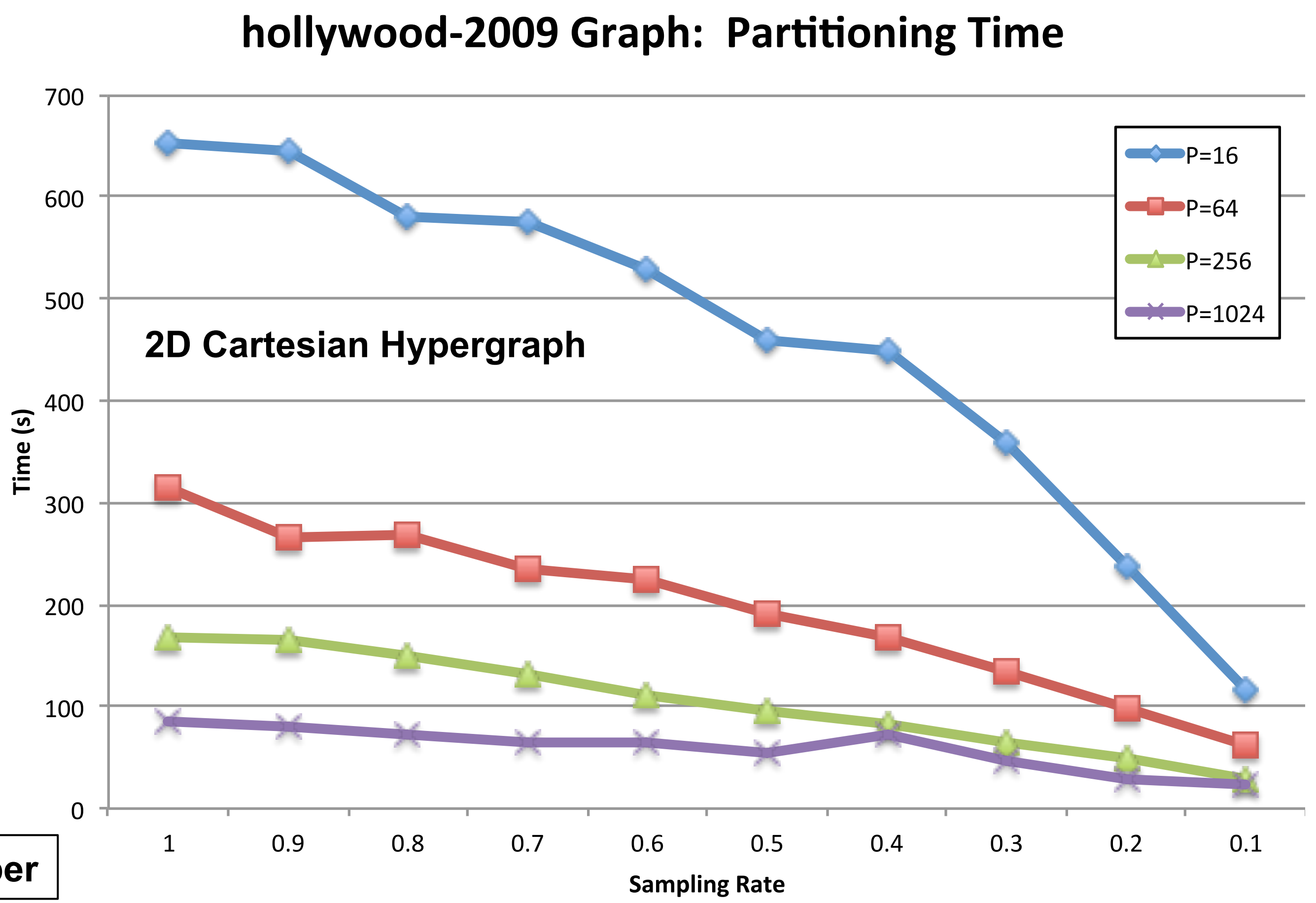


- Idea: Partition sampled graph to reduce partitioning time
- Steps:
  1. Produce smaller graph G' by sampling edges in graph G (uniform random sampling), keep vertices same
  2. Partition G' (2D Cartesian Hypergraph)
  3. Apply partition to G

Wolf, Miller: *2014 IEEE HPEC Proc.*

hollywood-2009* Graph



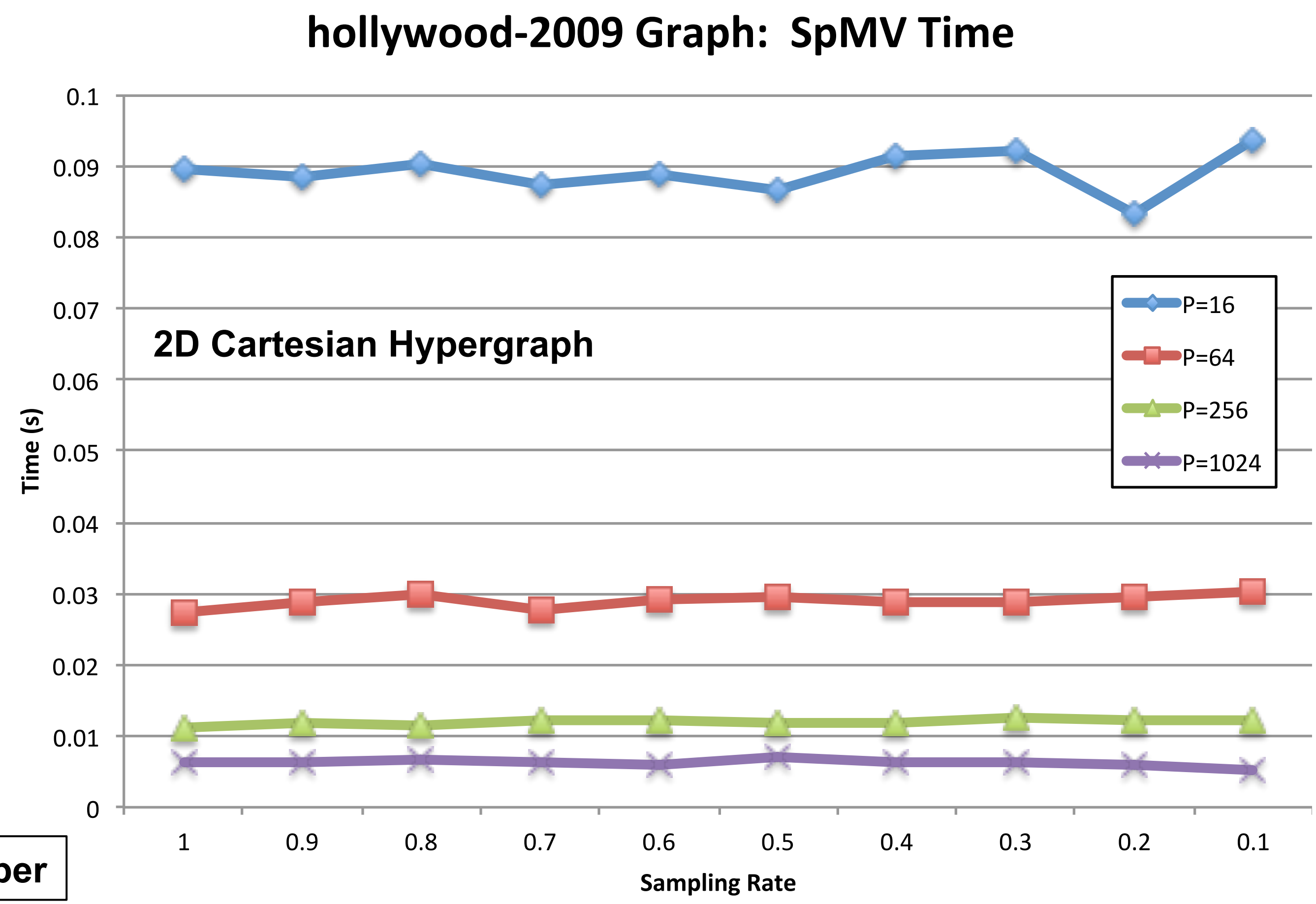
NERSC Hopper

Edge sampling greatly reduces partitioning time

*The University of Florida Sparse Matrix Collection

Wolf, Miller: *2014 IEEE HPEC Proc.*

hollywood-2009* Graph



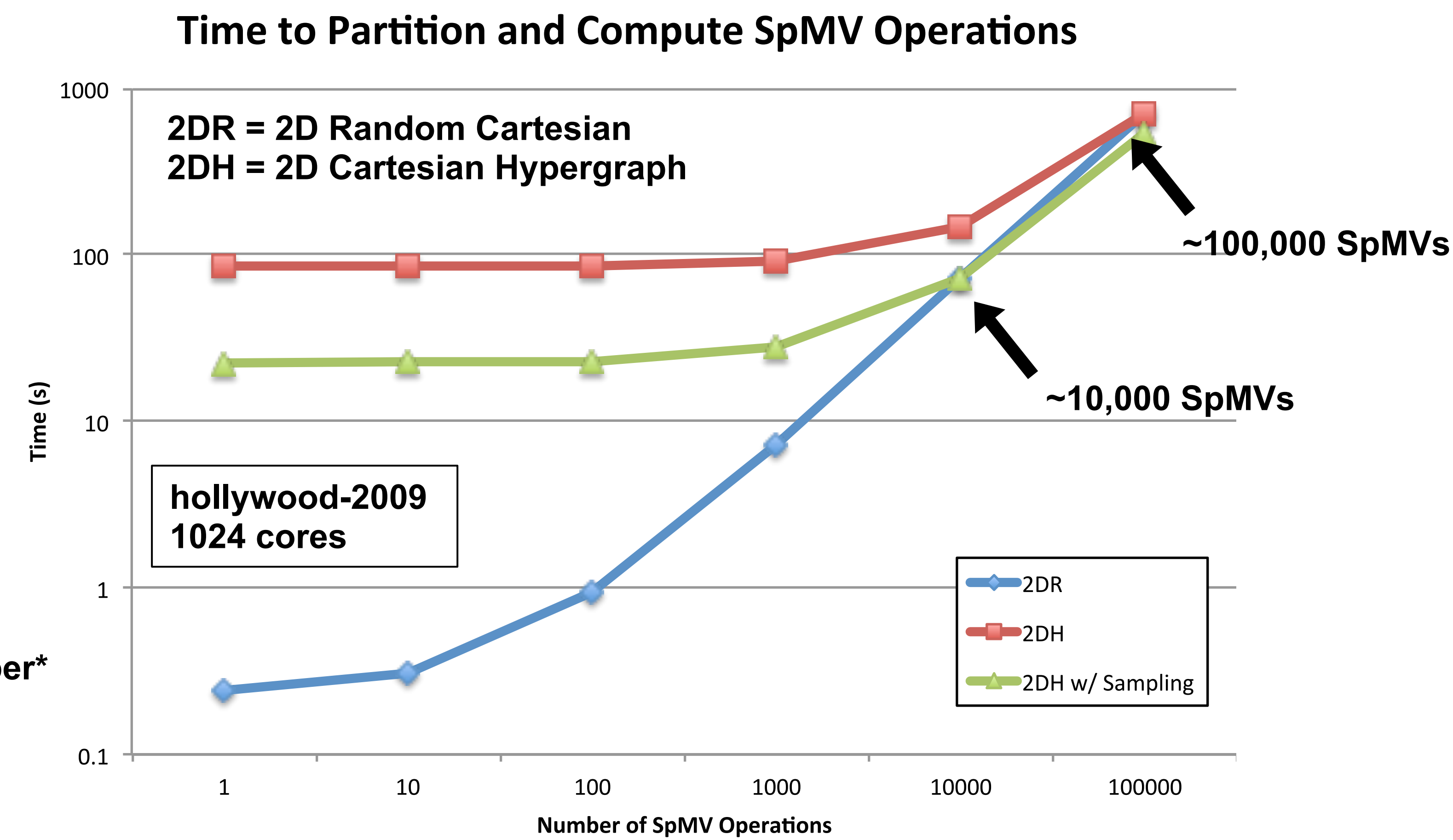
NERSC Hopper

Resulting SpMV time does not increase for modest sampling

*The University of Florida Sparse Matrix Collection

Wolf, Miller: *2014 IEEE HPEC Proc.*

Challenge with Hypergraph Partitioning Revisited



NERSC Hopper*

Sampling reduces overhead of hypergraph partitioning (fewer SpMVs needed to amortize partitioning cost)

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Wolf, Miller: *2014 IEEE HPEC Proc.*

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Summary

- Outlined HPC approach to processing big data
  - Signal processing for graphs
  - Statistical framework for anomaly detection in graphs
- Key component is eigensolver for dimensionality reduction
- Solving eigensystems resulting from power law graphs challenging
  - Load imbalance
  - Poor data locality
- SpMV key computational kernel
  - 1D data partitioning limits performance due to all-to-all communication
  - 2D data partitioning can be used to improve scalability
- Sampling can improve hypergraph-based partitioning performance for web/SN graphs

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- Sanjeev Mohindra (MITLL)
- Eddie Rutledge (MITLL)
- Scott Sawyer (MITLL)
- Matt Schmidt (MITLL)