

### INTRODUCTION

**Challenge:** Current IDR (iterative Krylov subspace) solver can be slower than Direct SuperLU for multi-RHS when forward modelling acoustic waves in Laplace-Fourier (LF) domain for 2nd and 4th order Finite-Difference (FD) discretization schemes.

**Objective:** Find a compromise of when direct SuperLU Solver is better than IDR and vice-versa:

- (1) Strong and weak scaling comparisons between the two solvers.
- (2) Maximum problem size that SuperLU can handle on fully packed nodes (default memory per core).
- (3) Advantages of using unpacked nodes (large memory per core) on Edison for SuperLU.

### GOVERNING EQUATIONS

The first-order system can be recast as a second-order equation in pressure after elimination of the particle velocities in the frequency-domain 3D acoustic first-order velocity-pressure system, that leads to a generalization of the Helmholtz equation:

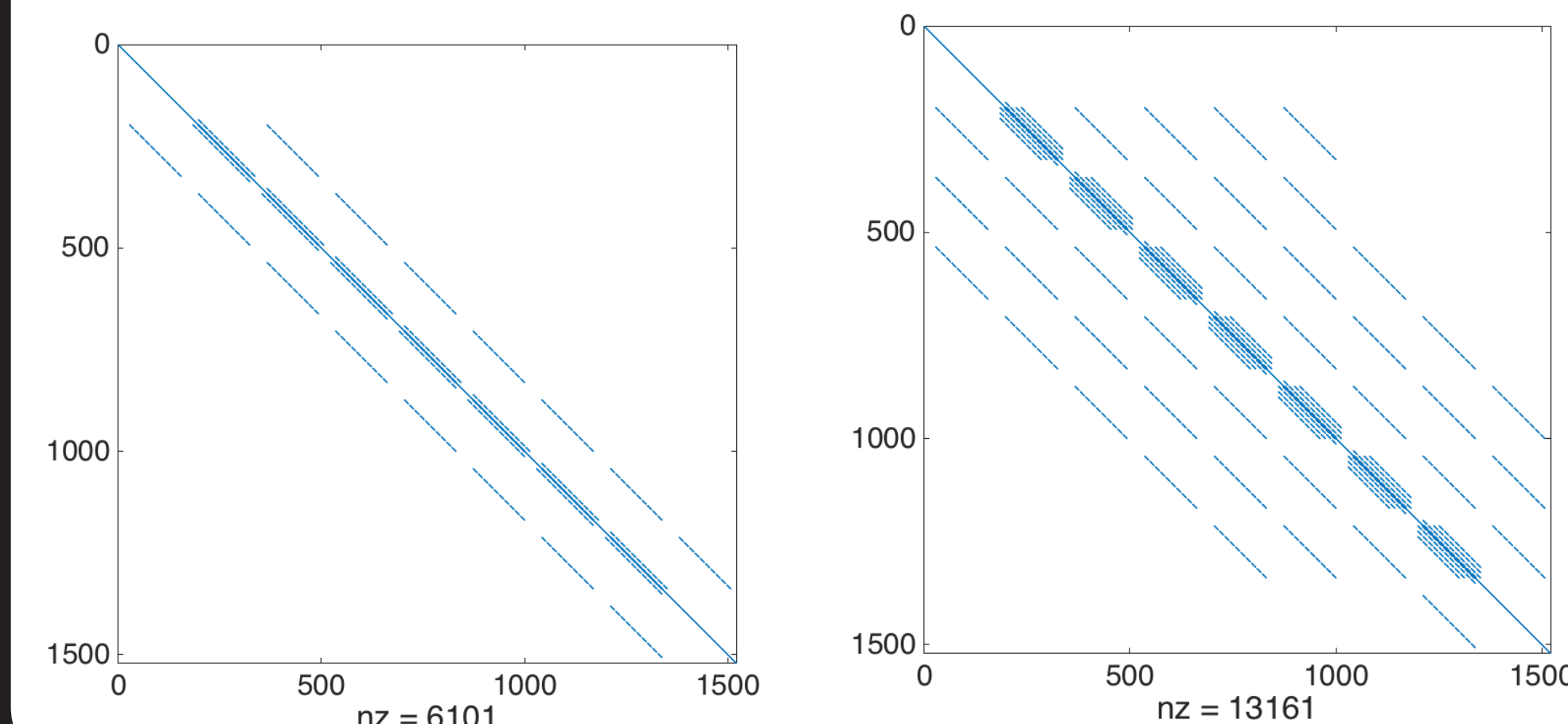
$$\frac{\omega^2}{\kappa(\mathbf{x})}p(\mathbf{x}, \omega) + \frac{\partial}{\partial x}b(\mathbf{x})\frac{\partial p(\mathbf{x}, \omega)}{\partial x} + \frac{\partial}{\partial y}b(\mathbf{x})\frac{\partial p(\mathbf{x}, \omega)}{\partial y} + \frac{\partial}{\partial z}b(\mathbf{x})\frac{\partial p(\mathbf{x}, \omega)}{\partial z} = s(\mathbf{x}, \omega). \quad (1)$$

Equation 1 can be recast in matrix form:

$$[\mathbf{M} + \mathbf{S}]\mathbf{u} = \mathbf{A}\mathbf{u} = \mathbf{b}. \quad (2)$$

### 2ND VS 4TH ORDER SCHEMES

**A** matrix for both second and fourth order schemes:



### REFERENCES

- [1] Li, Xiaoye S and Demmel, et. al On SuperLU user's guide In 2011.
- [2] Sonneveld, Peter and van Gijzen, Martin B On IDR (s): A family of simple and fast algorithms for solving large nonsymmetric systems of linear equations In 2008.

### PARALLEL SUPERLU ALGORITHM

```
for block K = 1 to N do
1 Factorize A(K : N, K) → L(K : N, K)
   (may involve pivoting)
2 Compute U(K, K + 1 : N)
   (via a sequence of triangular solves)
3 Update A(K + 1 : N, K + 1 : N) ←
  A(K + 1 : N, K + 1 : N) - L(K + 1 :
  N, K) · U(K, K + 1 : N)
   (via a sequence of calls to GEMM)
```

The algorithm is chosen for parallel SuperLU:

- (1) The sparsity structure can be determined before numerical factorization because of static pivoting.
- (2) All the GEMM (general matrix multiplication) updates to the trailing submatrix are independent and so can be done in parallel.

### SUPERLU PROS & CONS

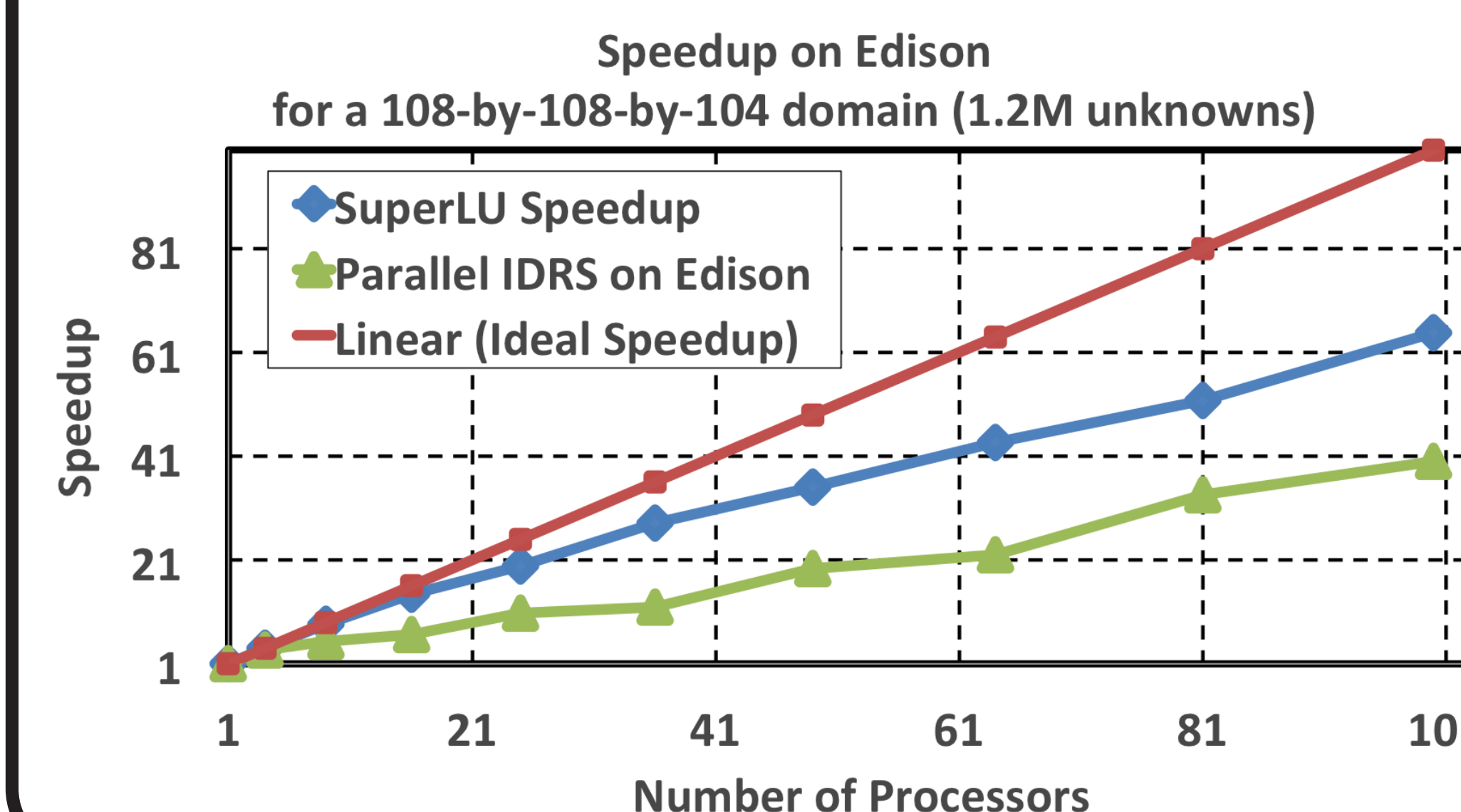
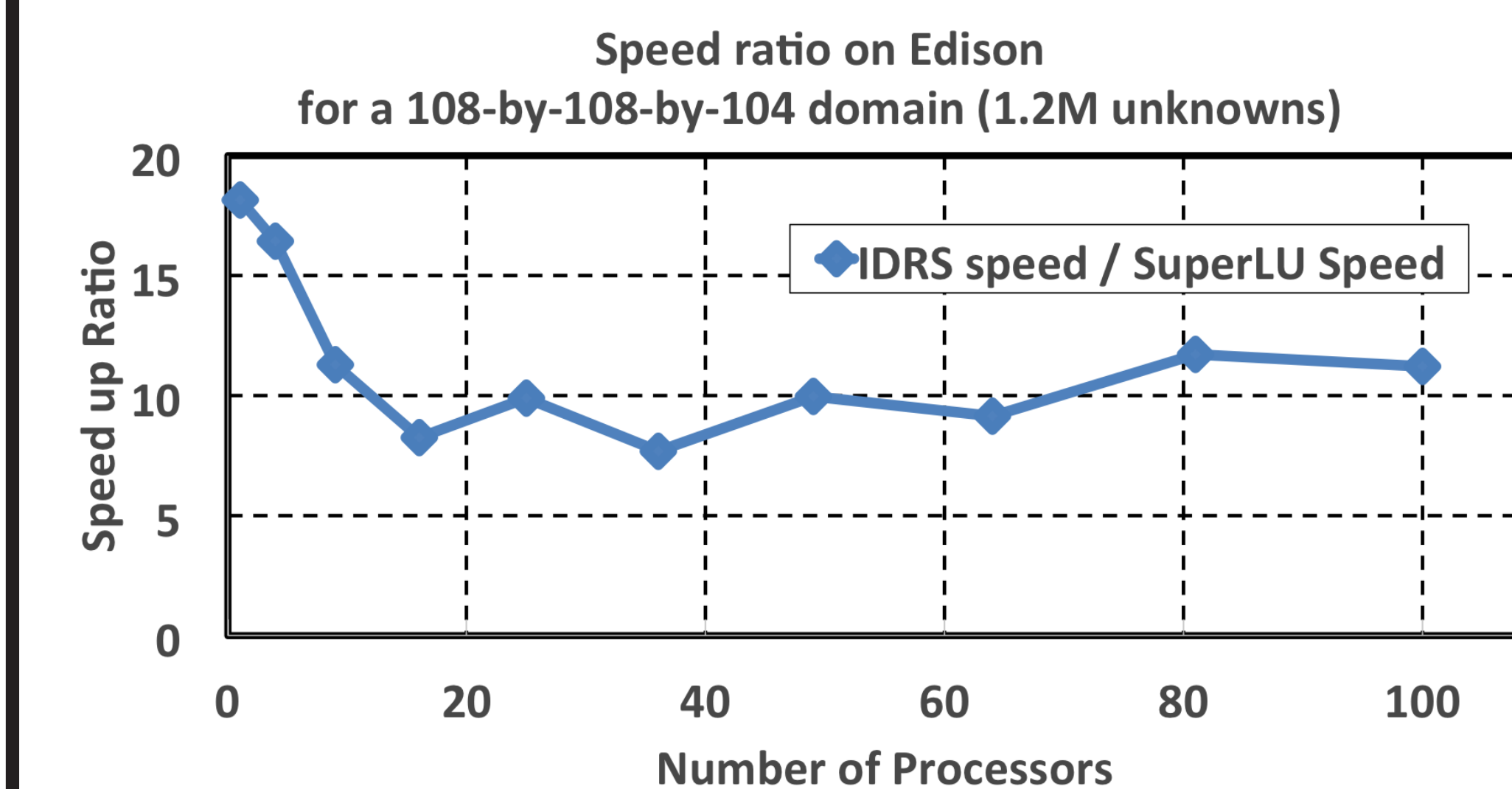
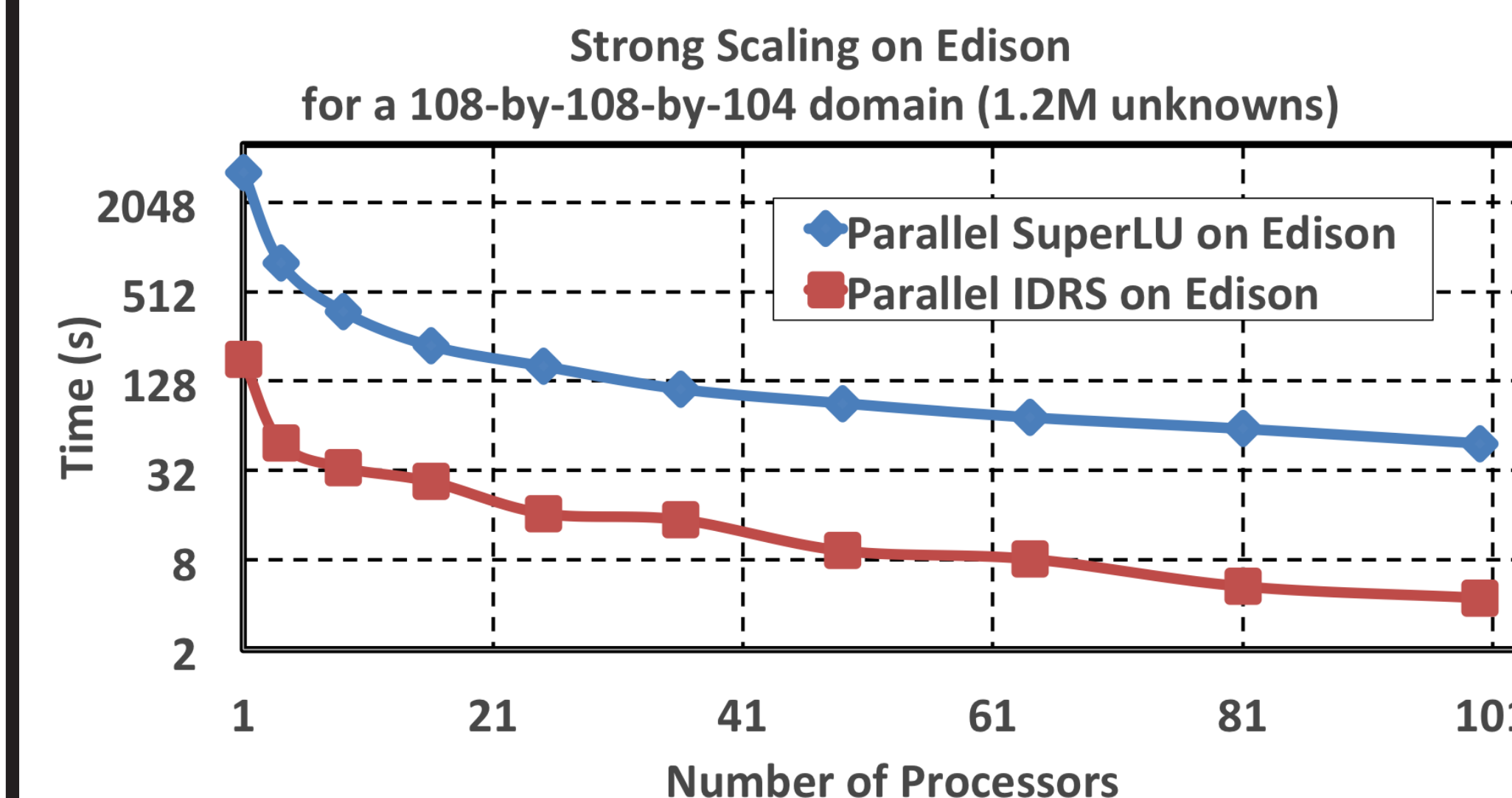
**Advantages** of using SuperLU:

- (1) Can solve for multiple RHS (sources) cheaply once matrix **A** is factorized.
- (2) Scales better when using multiple processors compared to the current IDR(s) method.

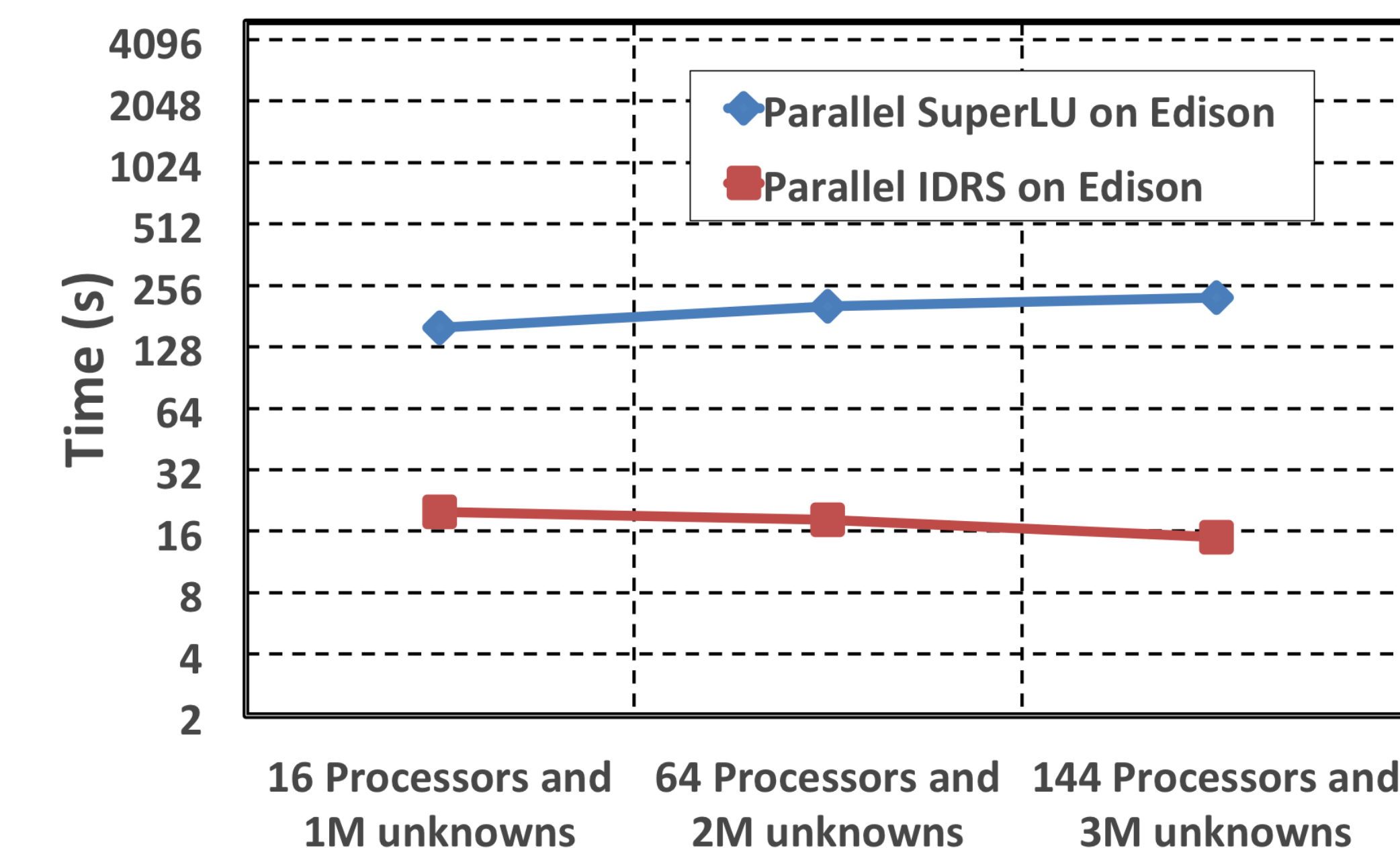
**Drawbacks** of using SuperLU:

- (1) Out of memory (OOM) errors during fill-in for large matrices.
- (2) SuperLU is generally slower than iterative methods when solving for one RHS.

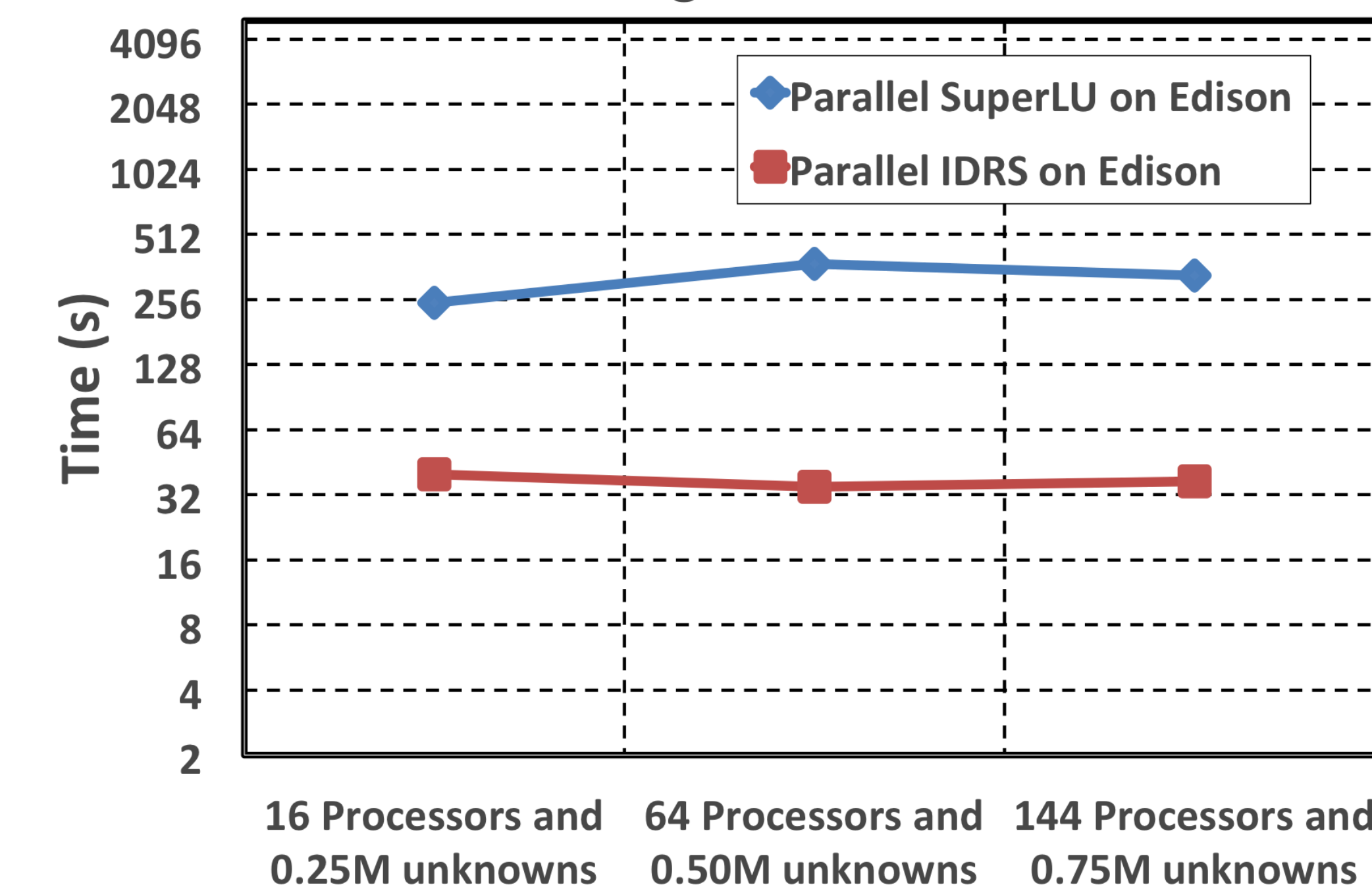
### PARALLEL RESULTS ON FULLY PACKED NODES



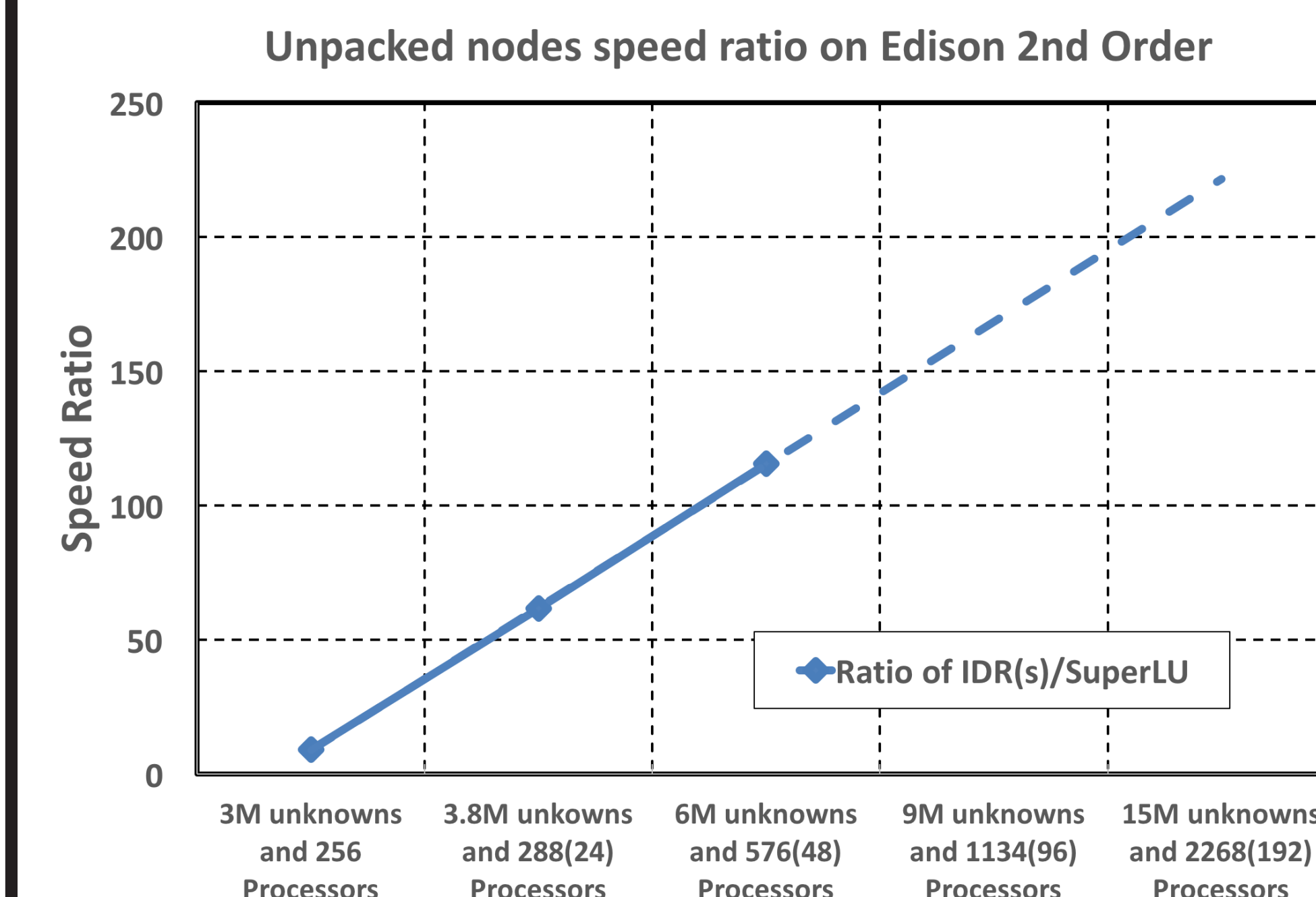
#### Weak Scaling in Edison 2nd Order



#### Weak Scaling in Edison 4th Order



### UNPACKED NODES RESULTS



### OBSERVATIONS

- (1) For medium-sized problems and using fully packed nodes (2.67GB per core), IDR(s) is 10 times faster than SuperLU.
- (2) For large-sized problems and using unpacked nodes (32GB per core), IDR(s) is 100 times faster than SuperLU.
- (3) SuperLU runs out of memory for medium-sized problems with fourth order discretization. Imagine the maximum size it can handle for elastic problems!
- (4) SuperLU is more efficient in strong-scaling.