Parallel Efficiency of the Lanczos Method for eigenvalue problems

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Outline

- Lanczos method
- efficiency of MATVEC
- efficiency of direct method
- overall efficiency

Eigenvalue problems

$$Ax = \lambda x$$

small matrices	large matrices
QR and variants	<u>projection based methods</u>
Jacobi method	trace minimization
twisted factorization	Newton method

commonly used projection methods: Lanczos, Arnoldi, Davidson

Lanczos algorithm

Major components of a Lanczos program

- Dense linear algebra operations:

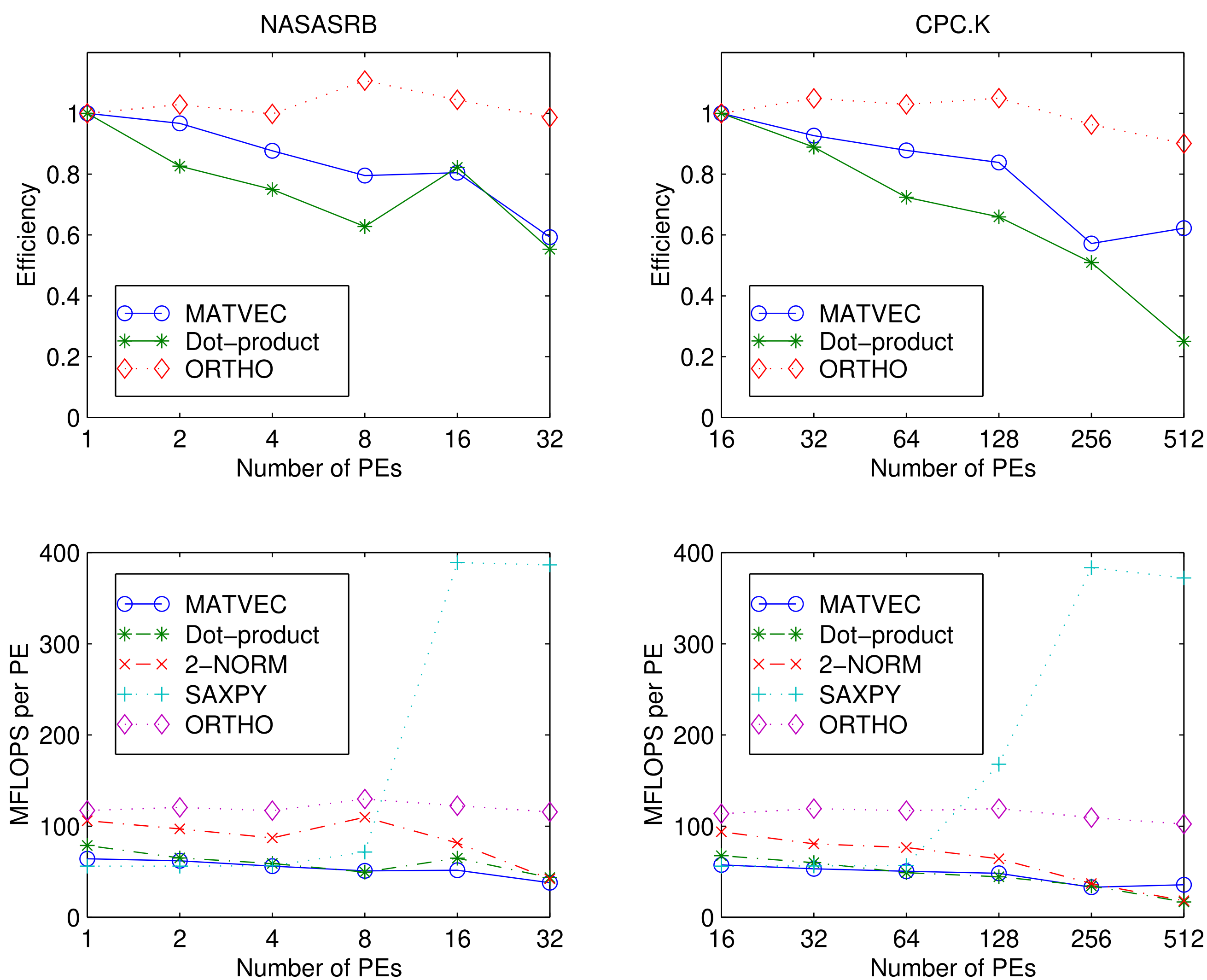
  dot-product,
  SAXPY,
  solve the projected eigenvalue problem, (restarting)
  re-orthogonalization

- Applying the operator

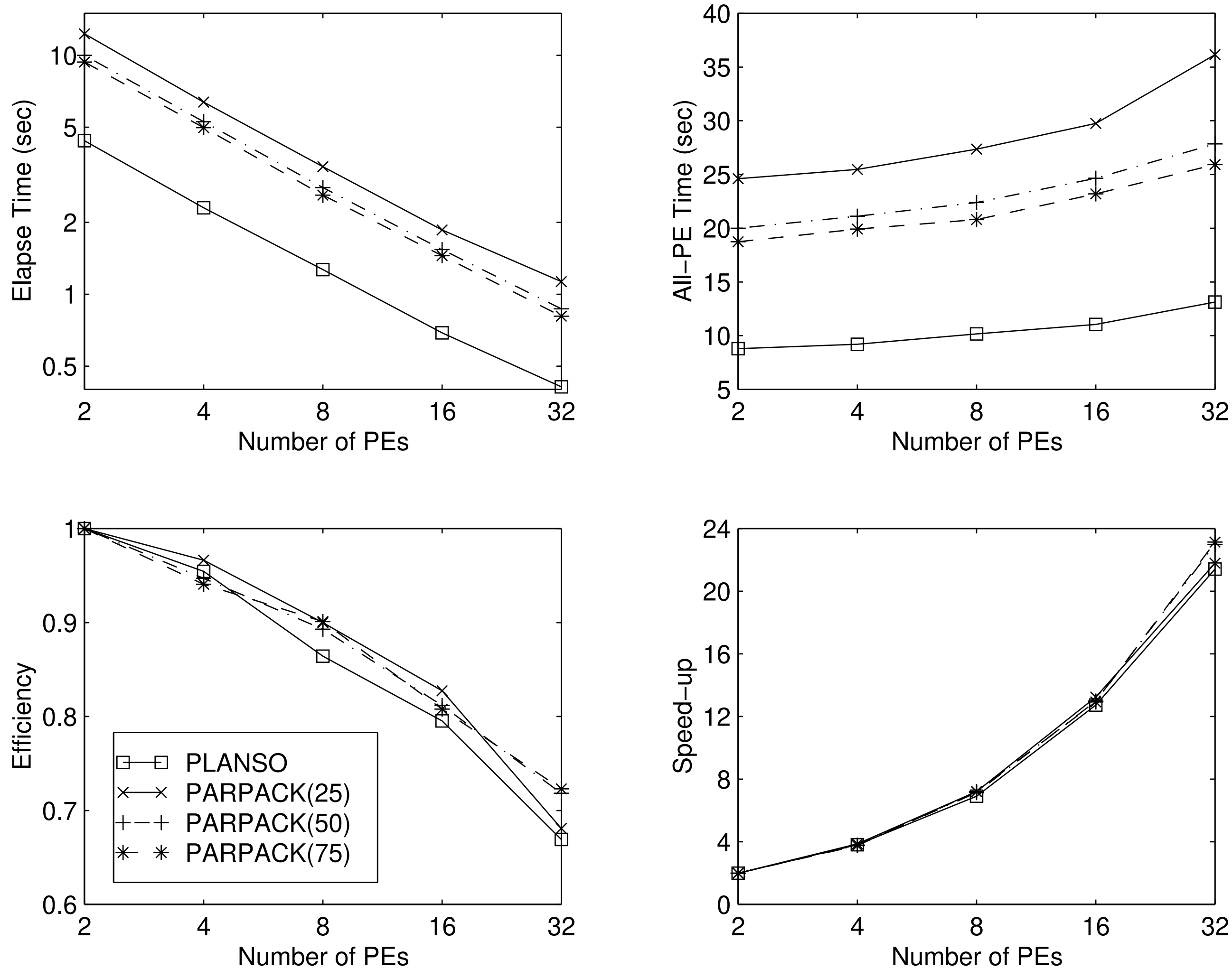
  directly applying the operator: A

  spectrum transformation: $(A - \sigma I)^{-1}$

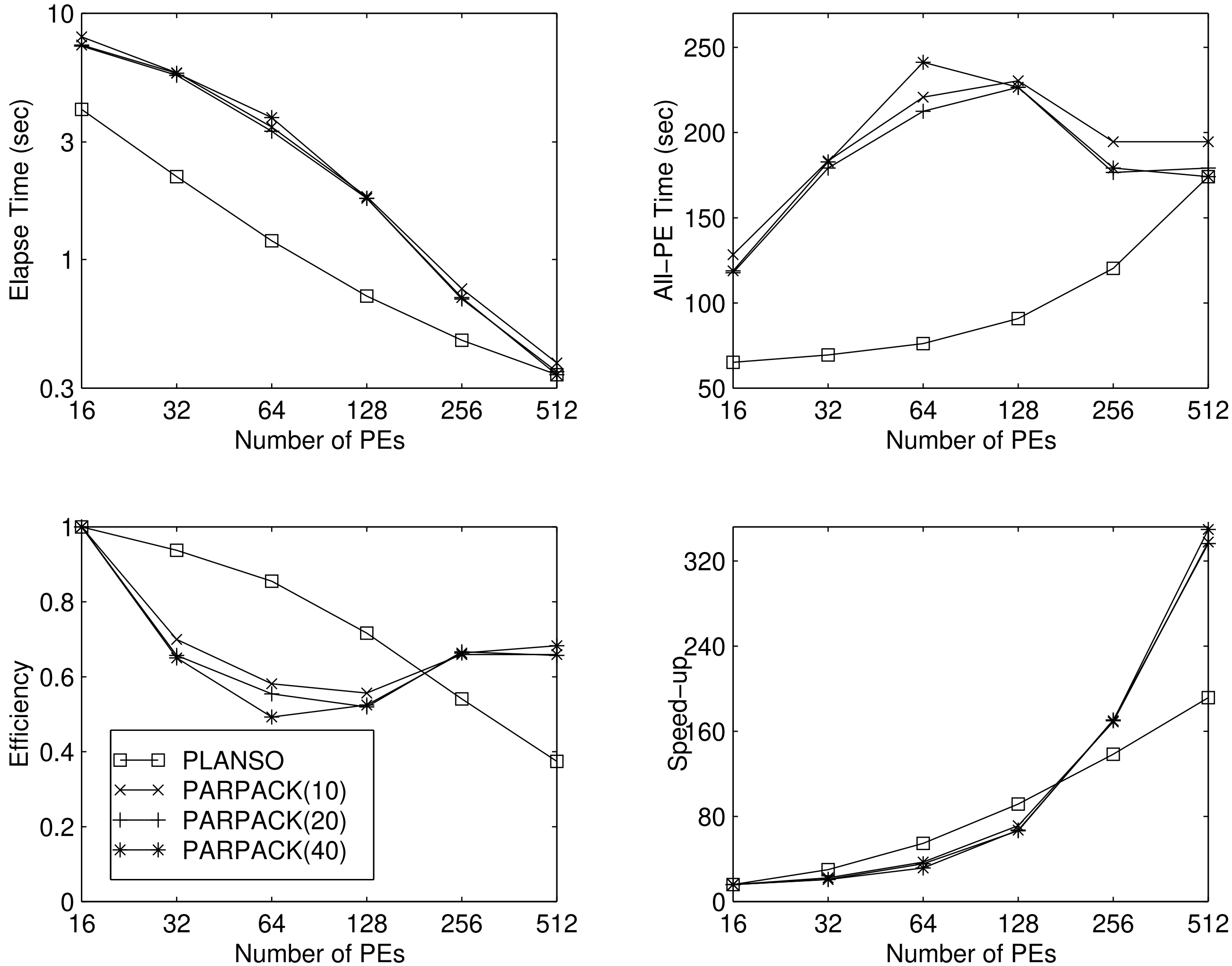
efficiencies of major components



NASASRB 54870x54870, NNZ 2677324



CPC.K 637244x637244, NNZ 30817002



a LU factorization example

n	1	2	4	8	16	32	64	128	256	512
34	74.4	41.5	23.5	14.3	9.9	8.3	6.8	6.5	6.8	6.9
40		101	56.1	32.5	21.8	16.7	14.1	12.9	13.1	13.4
48			152	87.1	55.5	40.3	32.4	29.2	28.1	
56				204	125	86.6	66.1	58.2		

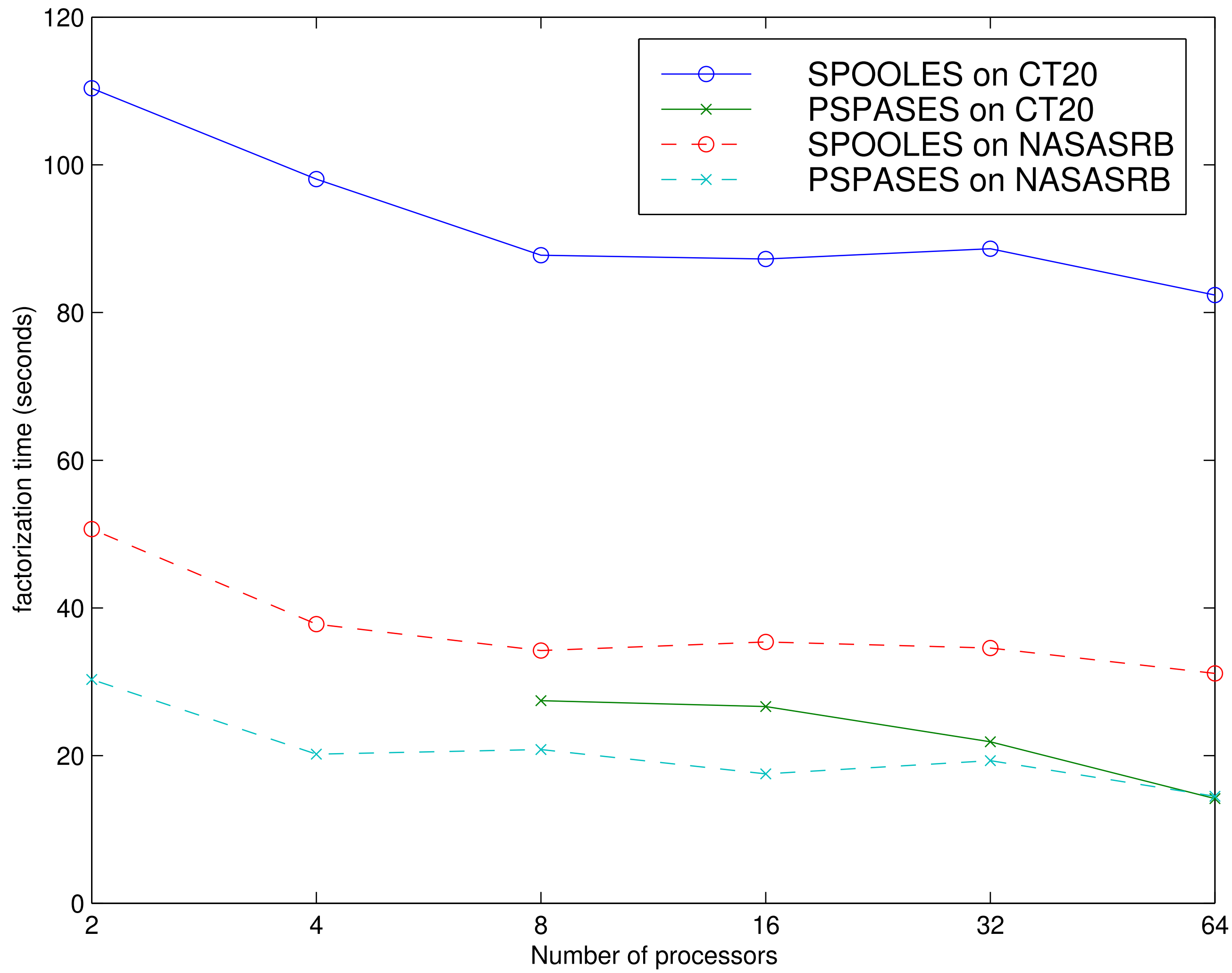
time (seconds) to factor 3-D 27-point stencil matrices on

a Cray T3E 900 using SPOOLES with MPI

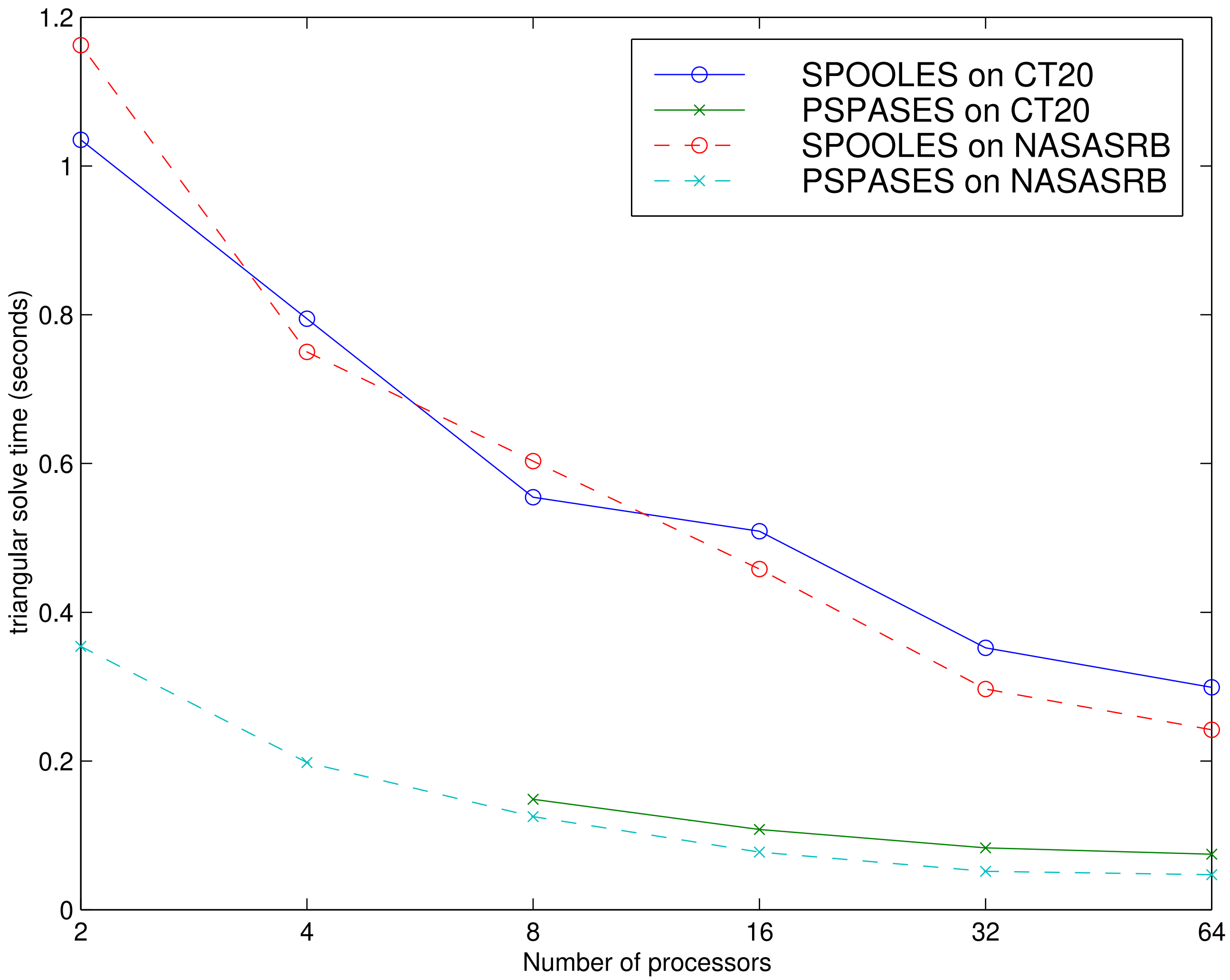
grid: $n \times n \times n$

number of processors: 1---512

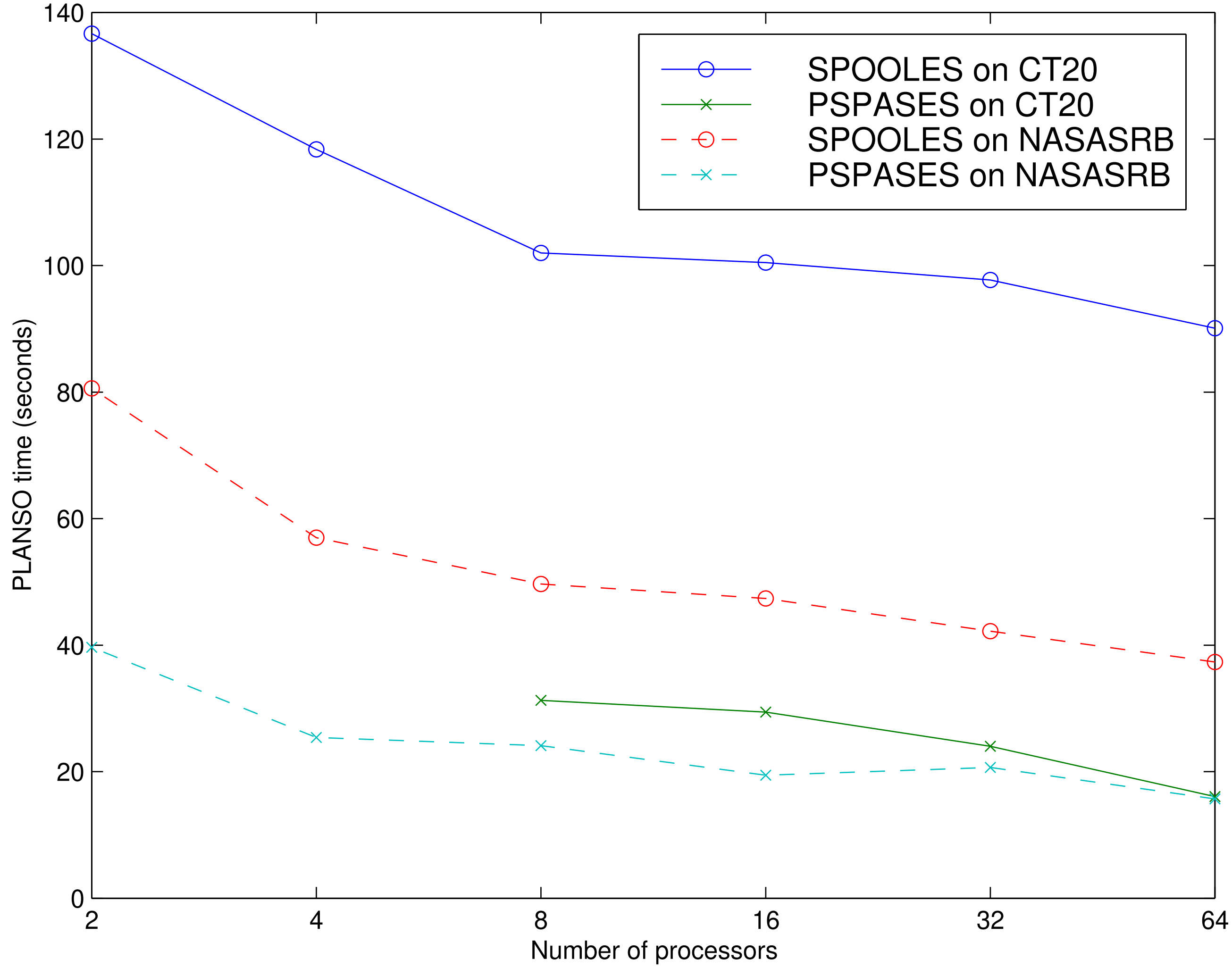
time to compute LU factors



time to perform one triangular solve



time to carry out 25 Lanczos iterations



to transform or not to transform

	no transform	shift-and-invert
iterations	50467	25
time (sec)	8546	50(SPOOLES) 24(PSPASES)

Time (seconds) to compute 5 smallest eigenvalues of NASASRB on 8 processors of a T3E 900

$$(\lambda_2 - \lambda_1)/(\lambda_{max} - \lambda_1) = 10^{-10}$$

$$\lambda_{max}/\lambda_1 = 6 \times 10^8$$

Scalability is important

If Lanczos method scales perfectly without spectrum transformation, how many processors are needed to catch up

1368 PEs to 50 seconds

2848 PEs to 24 seconds

Summary

- ✓ parallel direct solver packages are available now
- ✓ spectrum transformation techniques are effective
- ✓ shift-and-invert schemes does not scale as well as MATVEC
- → efficiencies the direct solvers will improve
- → alternative spectrum transformation schemes needed

http://www.nersc.gov/~kewu/pp99.html