The Solution of Large Dense Generalized Eigenvalue Problems on the CRAY X-MP/24 with SSD

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Properties of the Eigenvalue Problem

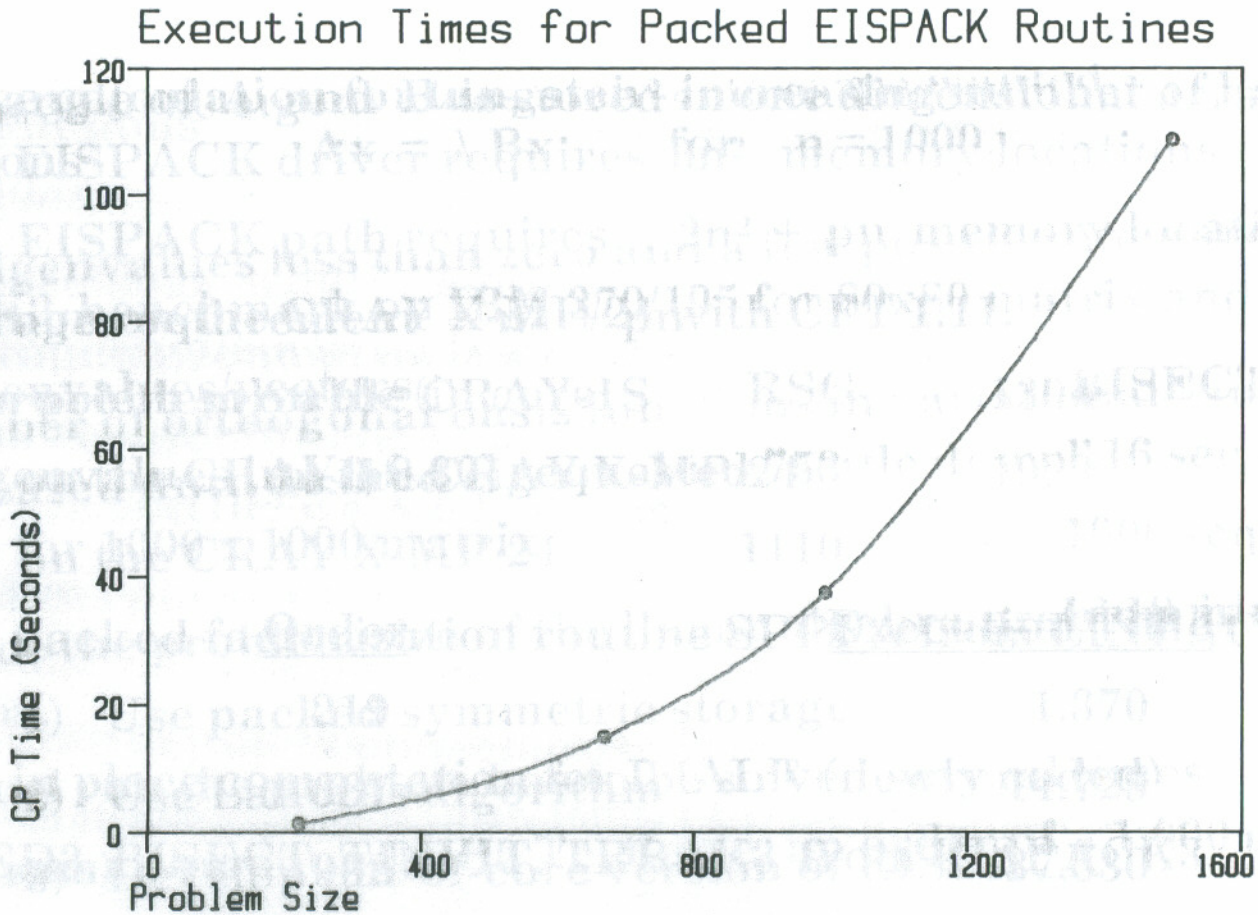
- About 30 to 50 eigenvalues and vectors are wanted.
- All eigenvalues less than zero and a few positive ones are needed.
- Number of orthogonal basis functions in variational "ansatz" are increased until desired eigenvalues "settle down".
- Hence the problem size of the linear algebra problem is not a known priori.
- For some compounds (Ba Te, Ba Se) an order of $\approx$ 1,000 is necessary.

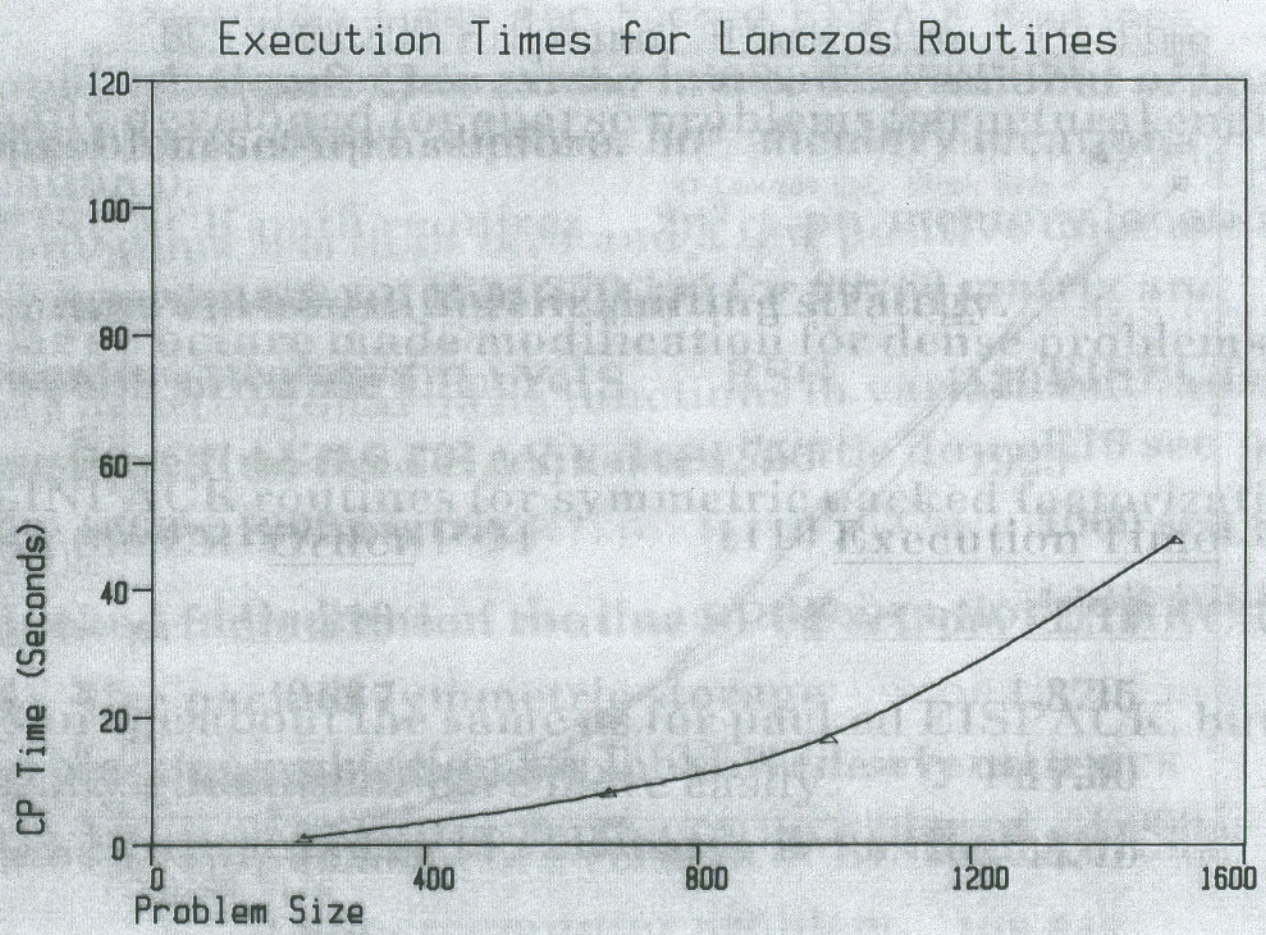
BCS - Block Shifted Lanczos Algorithm for $Ax = \lambda Bx$

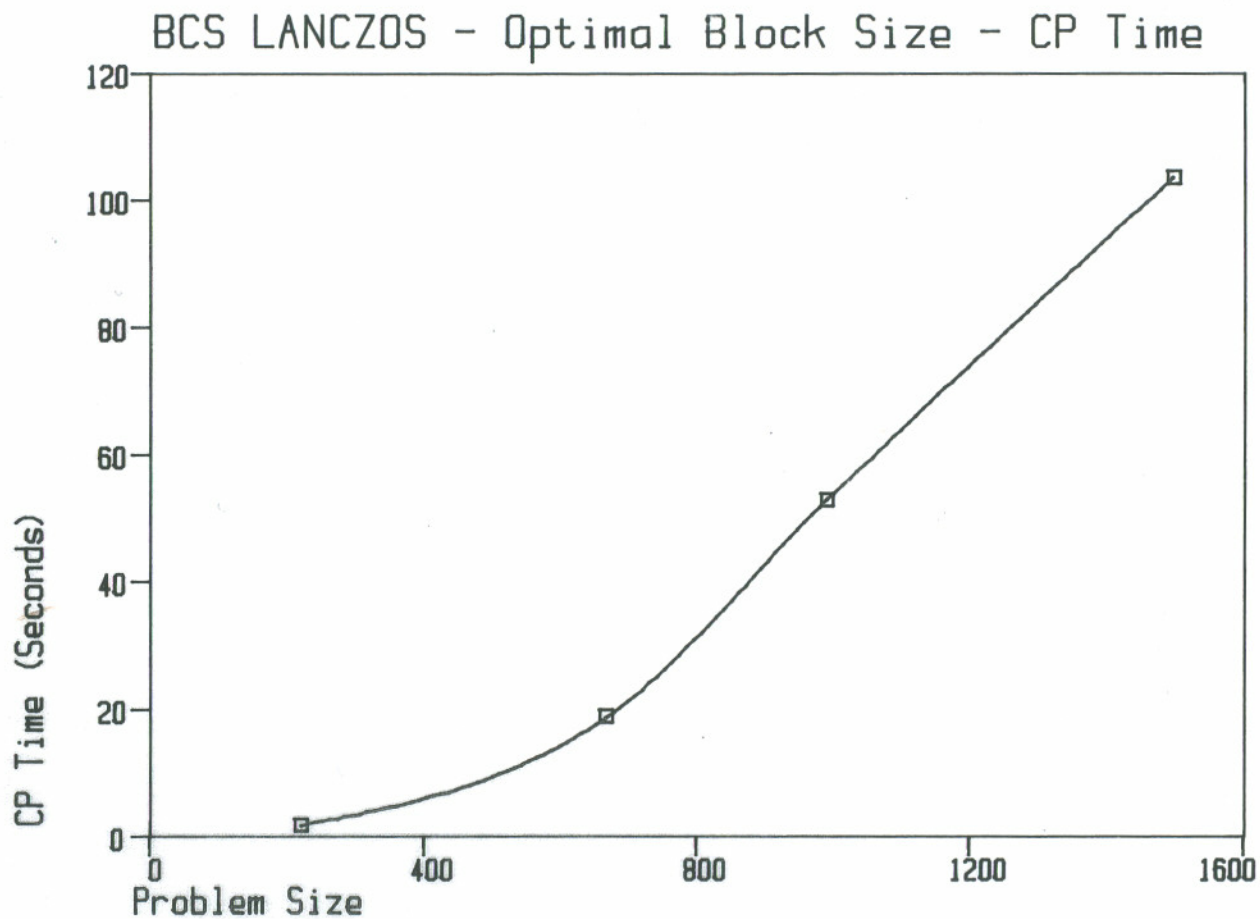
- Originally developed for sparse problems (structural engineering applications).
- Modular structure made modification for dense problems easy.
- Uses LINPACK routines for symmetric packed factorization (SSPCO).
- Total storage about the same as for packed EISPACK, but potentially goes out-of-core more easily.

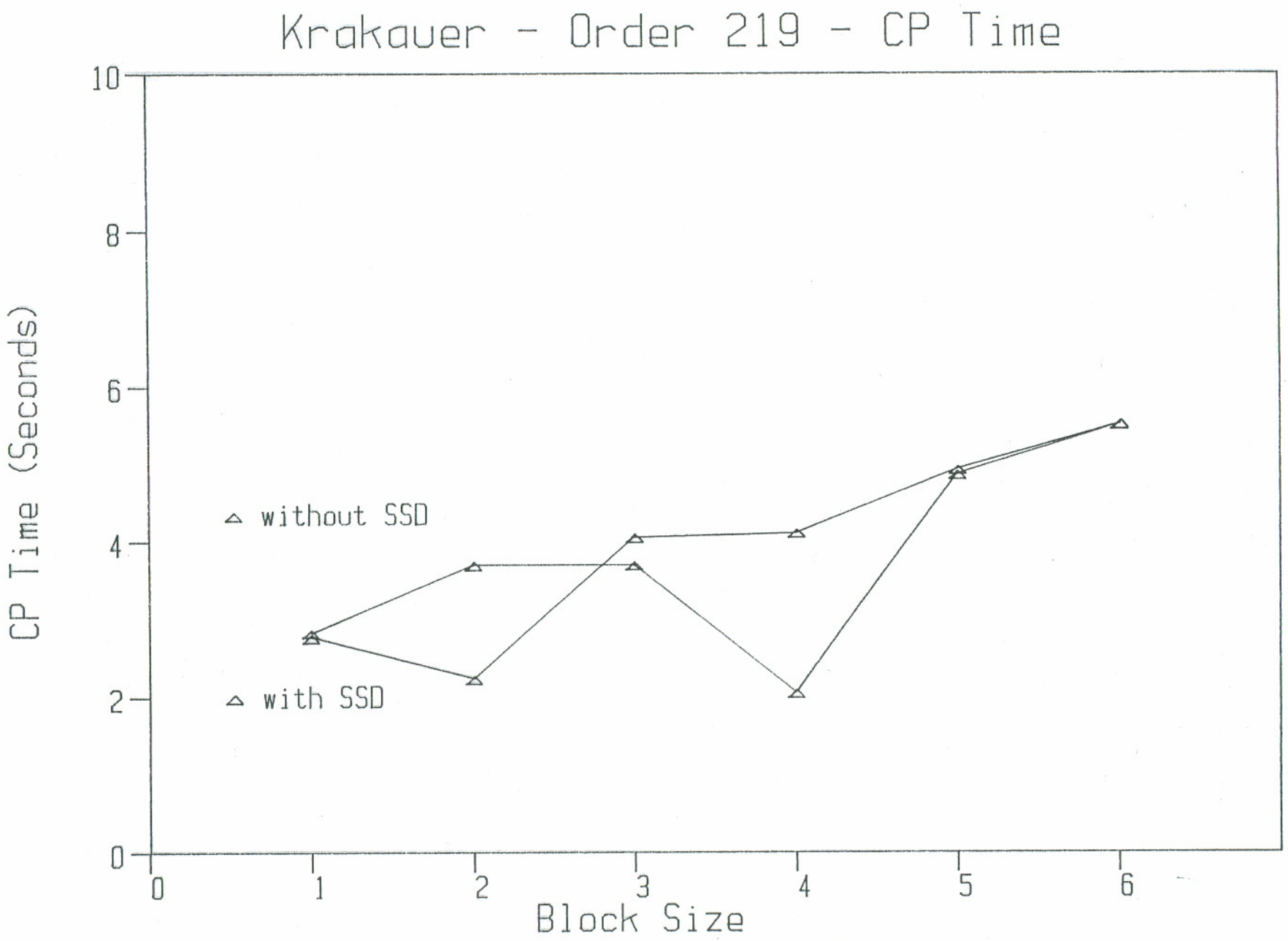
Conclusions

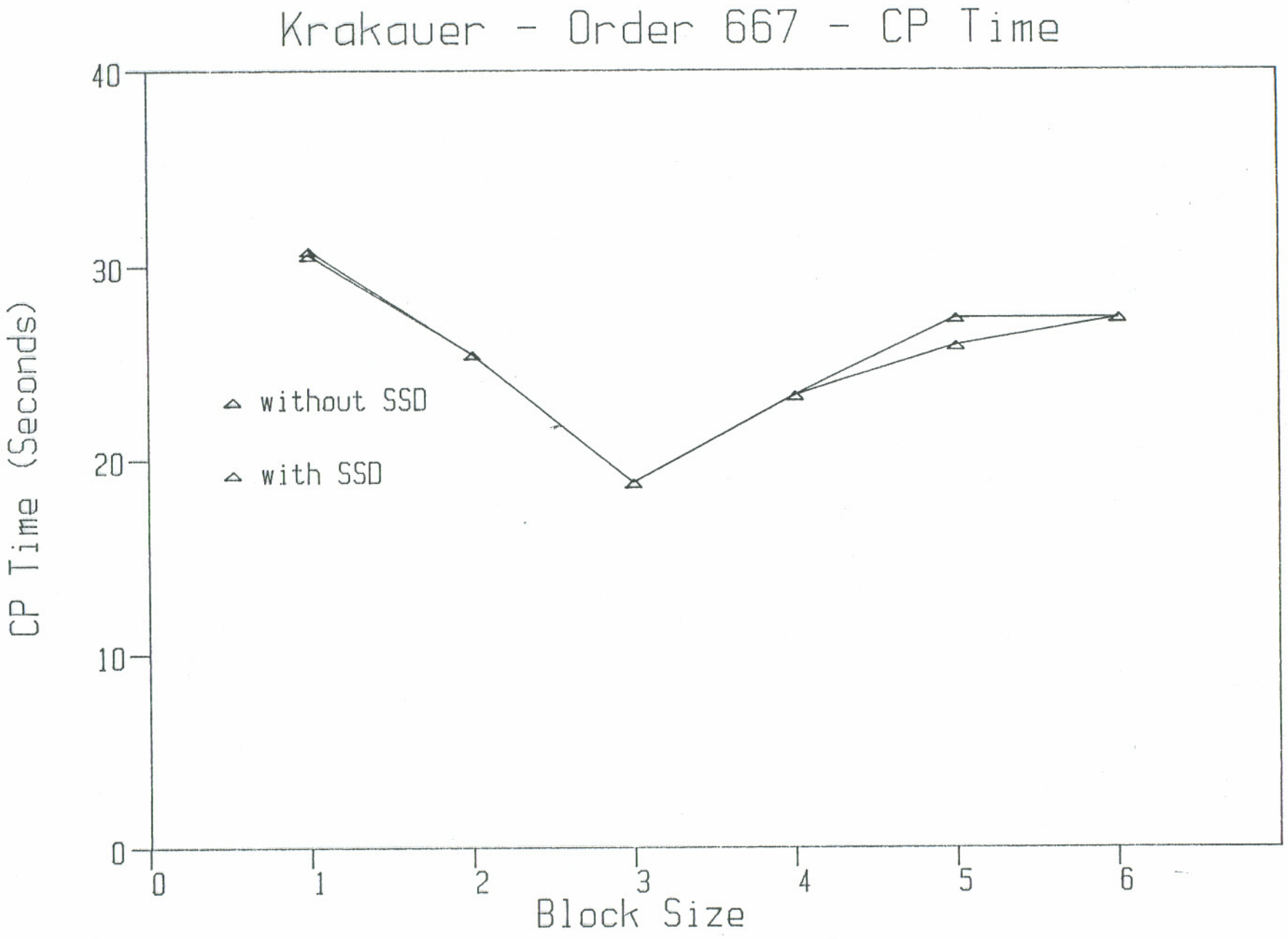
- Lanczos algorithm more efficient, even for dense problems.
- Lanczos more easily extended to an out-of-core version for larger problems.
- Standard software (EISPACK?) for large dense problem needed.
- Successful example of industry/academic cooperation in the framework of NSF Supercomputing initiative.

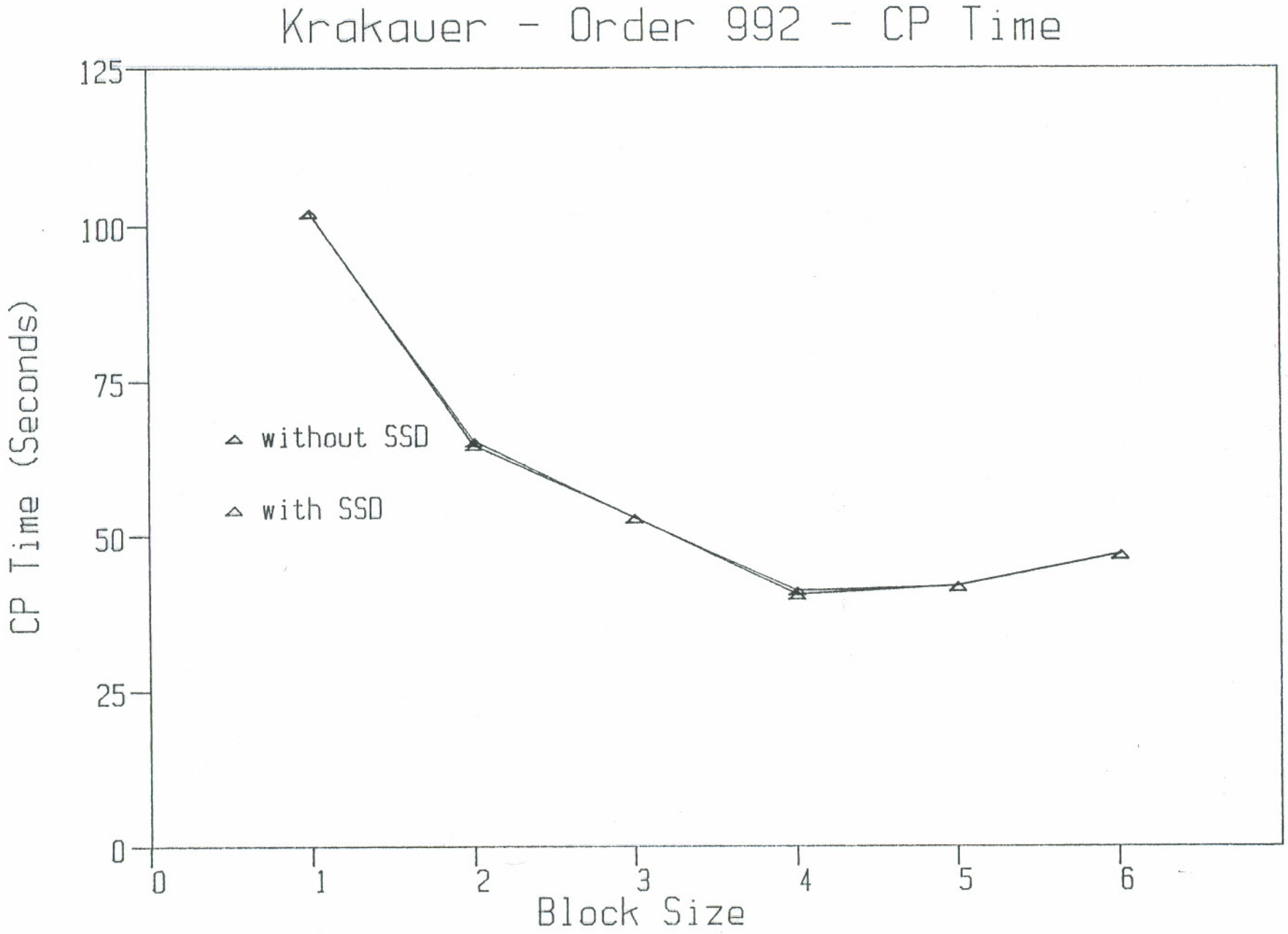

Execution Times for Packed EISPACK Routines
CP Time (Seconds)
0
20
40
60
80
100
120
0
400
800
1200
1600
Problem Size

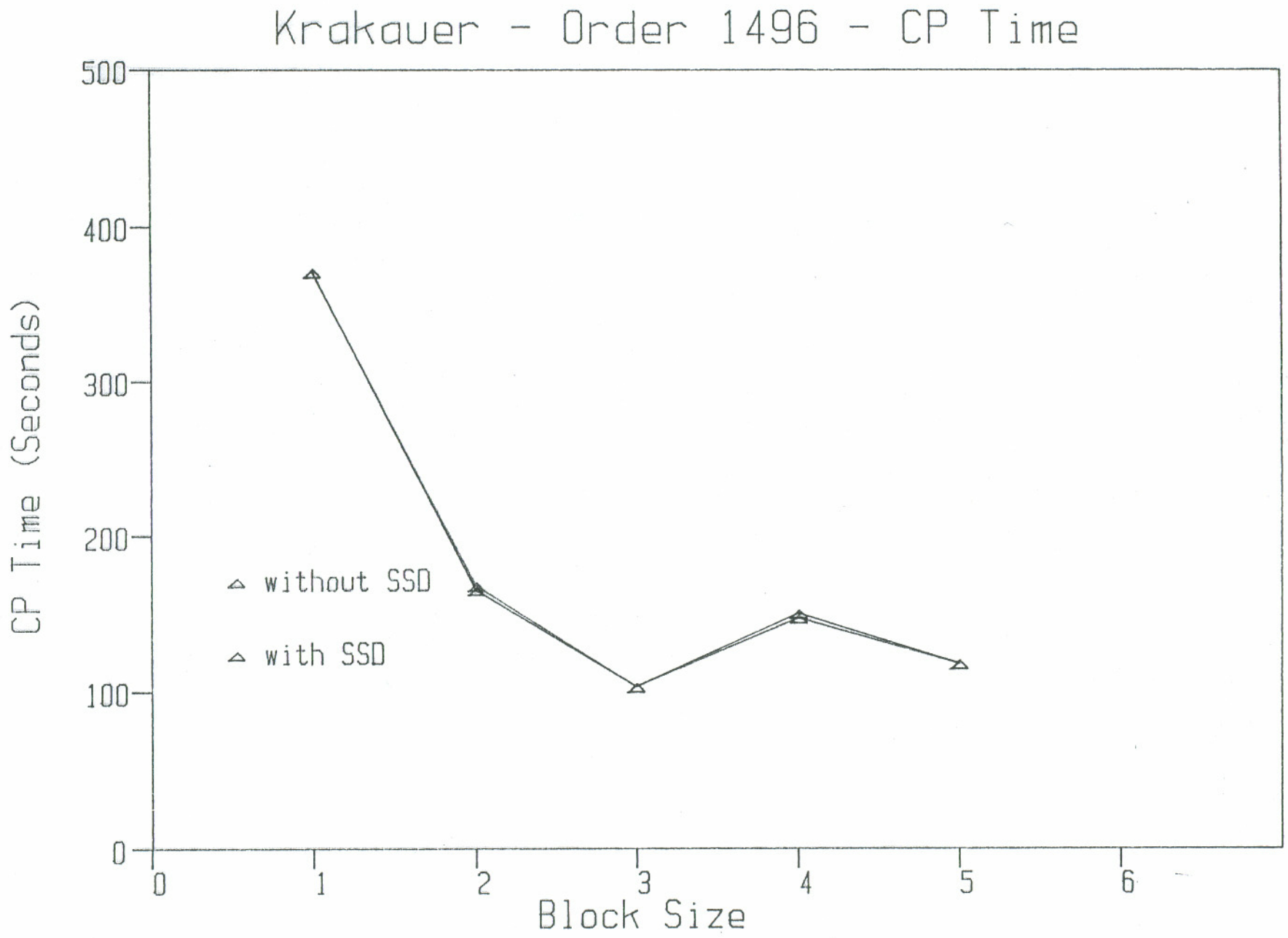

Execution Times for Lanczos Routines
CP Time (Seconds)
120
100
80
60
40
20
0
0
400
800
1200
1600
Problem Size

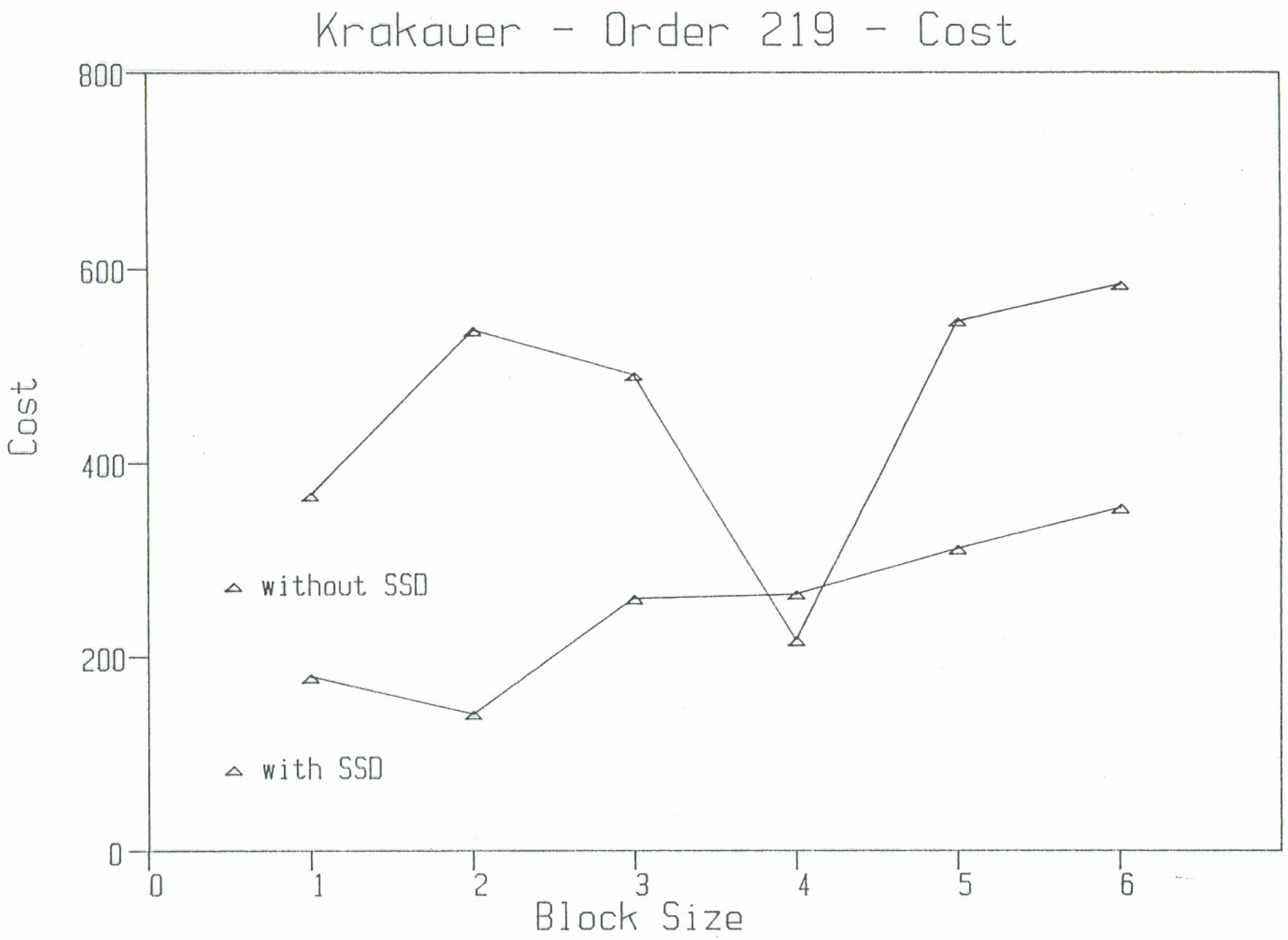

BCS LANCZOS - Optimal Block Size - CP Time
CP Time (Seconds)
120
100
80
60
40
20
0
0
400
800
1200
1600
Problem Size

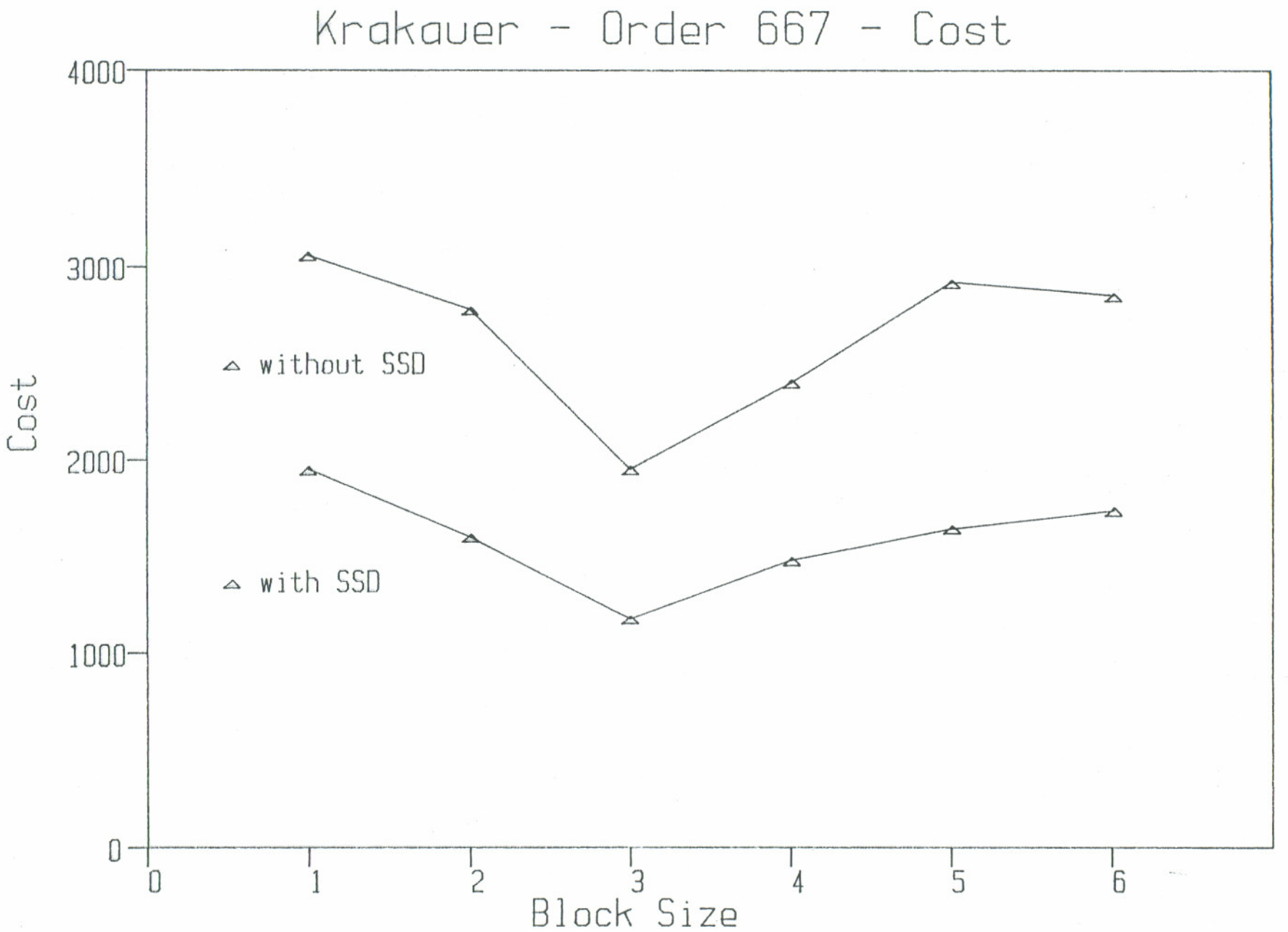

Krakauer - Order 219 - CP Time
CP Time (Seconds)
10
8
6
4
2
0
without SSD
with SSD
0
1
2
3
4
5
6
Block Size

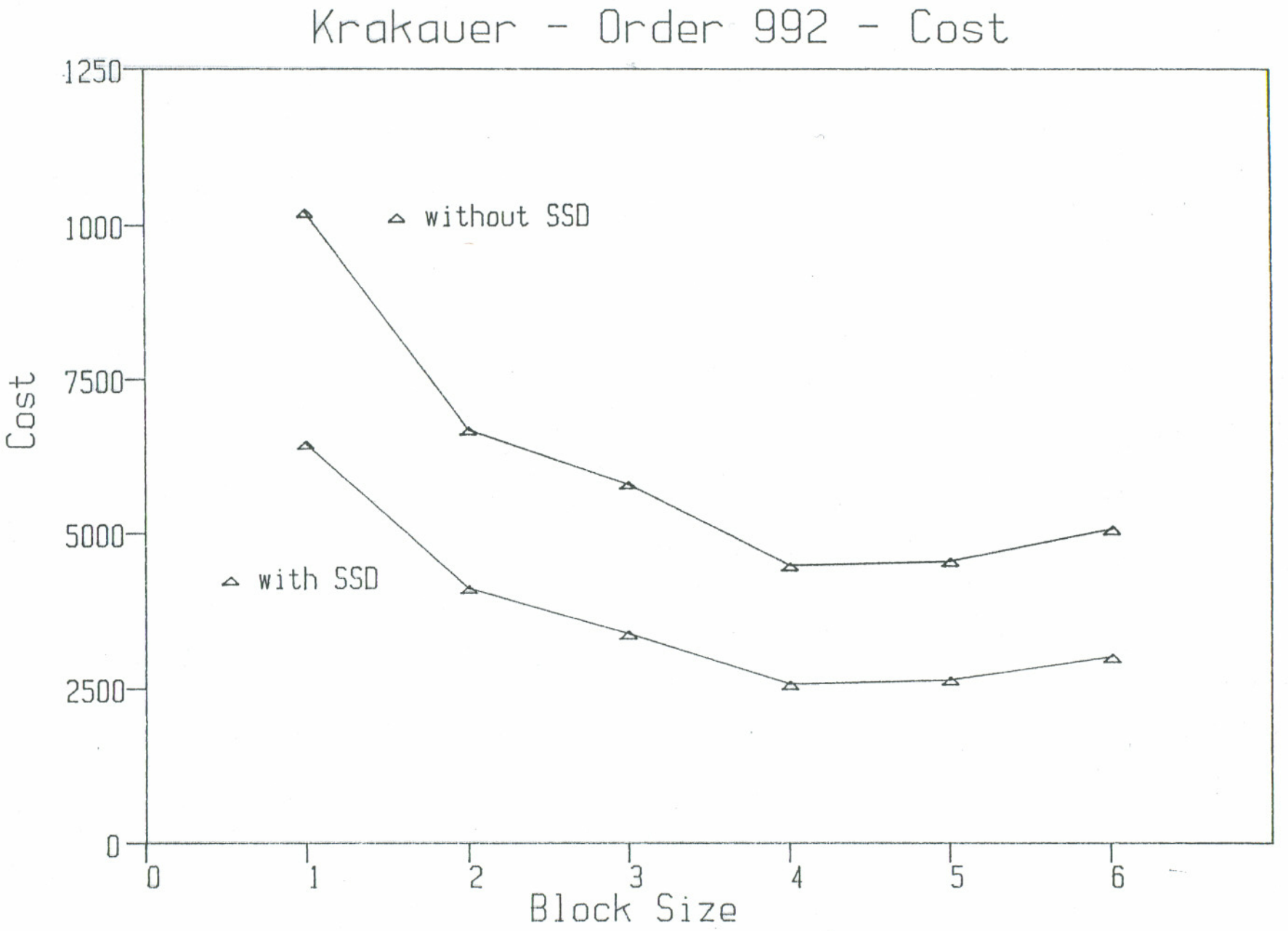

Krakauer - Order 667 - CP Time
CP Time (Seconds)
40
30
20
10
0
without SSD
with SSD
0
1
2
3
4
5
6
Block Size


Krakauer - Order 992 - CP Time
125
100
75
50
25
0
CP Time (Seconds)
without SSD
with SSD
0
1
2
3
4
5
6
Block Size


Krakauer - Order 1496 - CP Time
CP Time (Seconds)
500
400
300
200
100
0
without SSD
with SSD
0
1
2
3
4
5
6
Block Size


Krakauer - Order 219 - Cost
800
600
400
200
0
Cost
0
1
2
3
4
5
6
Block Size
without SSD
with SSD


Krakauer - Order 667 - Cost
4000
3000
2000
1000
0
Cost
without SSD
with SSD
0
1
2
3
4
5
6
Block Size


Krakauer - Order 992 - Cost
1250
1000
7500
5000
2500
0
Cost
without SSD
with SSD
0
1
2
3
4
5
6
Block Size

Krakauer - Order 1496 - Cost
6000
4500
3000
1500
0
Cost
without SSD
with SSD
0
1
2
3
4
5
6
Block Size