

CUSTOMIZE YOUR WORLD

Anslys Solvers Team, April, 2002

Outline



- Basic solver descriptions
 - Direct and iterative methods
 - *Why so many choices?*
- Solver usage in ANSYS
 - Available choices and defaults
 - *How do I chose a solver?*
- Practical usage considerations
 - Performance issues
 - Usage rules of thumb
 - Usage examples
 - *How do I chose the fastest solver??*

Solver Basics: $Ax = b$



Direct Methods

Factor: $A = LDL^T$

$$\begin{bmatrix} \blacksquare \end{bmatrix} = \begin{bmatrix} \blacktriangleleft & & \\ & \square & \\ & & \blacktriangleright \end{bmatrix}$$

Solve:

$$Lz = b \quad \begin{bmatrix} \blacktriangleleft \end{bmatrix} \mid = \mid$$

$$z = D^{-1}z \quad \begin{bmatrix} \square \end{bmatrix} \mid = \mid$$

$$L^T x = z \quad \begin{bmatrix} \blacktriangleright \end{bmatrix} \mid = \mid$$

Compute matrix L

Solve triangular systems

Solver Basics: $Ax = b$



Direct Methods

Factor: $A = LDL^T$



Solve:

$$Lz = b \quad \begin{array}{|c|} \hline \text{Lower triangular} \\ \hline \end{array} =$$

$$z = D^{-1}z \quad \begin{array}{|c|} \hline \text{Diagonal} \\ \hline \end{array} =$$

$$L^T x = z \quad \begin{array}{|c|} \hline \text{Upper triangular} \\ \hline \end{array} =$$

Compute matrix L

Solve triangular systems

Iterative Methods

Stationary Methods
(Guess and Go)

Choose x^0

Iterate:

$$x^{k+1} = Gx^k + c$$

Until

$$\|x^{k+1} - x^k\| < \epsilon$$

Compute sparse Ax product

Vector updates

Projection Methods
(project and minimize)

Choose x^0 ; $r^0 = Ax^0 - b$; $p^0 = r^0$

Iterate:

Compute Ap^k ;

$$\text{Update } x^k = x^{k-1} + \alpha^k p^{k-1}$$

$$r^k = r^{k-1} - \alpha^k Ap^k$$

$$p^k = r^k + \beta^k p^{k-1}$$

Until $\|r^k\| < \epsilon$

Solver Basics: Limitations



Direct Methods

- Factor is expensive
 - Memory & lots of flops
 - huge file to store L
- Solve I/O intensive
 - forward/backward read of huge L file

Iterative Methods

- Sparse Ax multiply cheap but slow
 - Memory bandwidth and cache limited
 - Harder to parallelize
- Preconditioners are not always robust
- Convergence is not guaranteed

ANSYS Direct Advantage



- Enhanced BCSLIB version 4.0
 - Parallel factorization
 - Reduced memory requirements for equation reordering
 - Support for U/P formulation
- Sparse solver interface improvements
 - Dynamic memory uses feedback for optimal I/O performance
 - Sparse assembly including direct elimination of CEs

Multi-Point Constraints



Direct elimination method

$$\mathbf{x}_1 = \mathbf{G}^T \mathbf{x}_2 + \mathbf{g}$$

A_{11}	A_{12}	$=$	x_1	b_1
A_{12}^T	A_{22}		x_2	b_2

solve :

$$(\mathbf{G}\mathbf{A}_{11}\mathbf{G}^T + \mathbf{G}\mathbf{A}_{12} + \mathbf{A}_{12}^T\mathbf{G}^T + \mathbf{A}_{22}) \mathbf{x}_2 = \mathbf{b}_2 + \mathbf{G}\mathbf{b}_1 - \mathbf{A}_{12}^T\mathbf{g} - \mathbf{G}\mathbf{A}_{11}\mathbf{g}$$

ANSYS Iterative Advantage



- Powersolver has a proprietary and robust preconditioner
 - Parallel matrix/vector multiply
 - Wide usage, robust
- Many additional iterative solvers for complex systems, non-symmetric, etc.
- New high performance parallel solvers
 - AMG Algebraic Multigrid
 - DDS Domain Decomposition Solver
- Ongoing efforts to utilize and enhance AMG and DDS solvers when applicable

Solver Usage



- Sparse, PCG and ICCG solvers cover 95% of all ANSYS applications
- Sparse solver is now default in most cases for robustness and efficiency reasons

Solver Usage: Choices



- Sparse direct solver (BCSLIB)
- PCG solver (PowerSolver)
- Frontal solver
- ICCG
- JCG

Listed by order of usage popularity

ANSYS now chooses sparse direct in nearly all applications for robustness and efficiency

Solver Usage: -pp Choices



- AMG – Algebraic Multigrid
 - Good for ill-conditioned problems
 - Best ANSYS shared memory parallel performance iterative solver
 - Good for nonlinear problems – can solve indefinite matrix
- DDS – Domain Decomposition Solver
 - Exploits MPP cluster computing for solver portion of analysis
 - Solver time scales even on many processors

Still under intensive developments

Solver Usage: Sparse Solver



- Real and complex, symmetric and non-symmetric
- Positive definite and indefinite(occurs in nonlinear and eigensolver)
- Supports block Lanczos
- Supports substructural USE pass
- Substructure Generation pass (Beta in 6.1)
- Supports ALL physics including some CFD
- Large numbers of CEs
- Support for mixed U-P formulation with Lagrange multipliers (efficient methods are used to support this)
- Pivoting and partial pivoting (EQSLV,sparse,0.01,-1)

Solver Usage: PCG Solver



- Real symmetric matrices
- Positive definite and indefinite matrices. Supporting indefinite matrices is a unique feature in our industry.
- Power Dynamics modal analyses based on PCG + subspace
- Substructure USE pass and expansion pass
- All structural analyses and some other field problems
- Large numbers of CEs
- NOT for mixed U-P formulation Lagrange multiplier elements
- NO pivoting or partial pivoting capability

Solver Usage: ICCG Suite



- Collection of iterative solvers for special cases
- Complex symmetric and non-symmetric systems
- Good for multiphysics, i.e. EMAG
- Not good for general usage

Usage Guidelines: Sparse



- **Capabilities**

- Adapts to memory available
- ANSYS interface strives for optimal I/O memory allocation
- Uses machine tuned BLAS kernels that operate at near peak speed
- Uses ANSYS file splitting for very large files
- Parallel performance 2X to 3.5X faster on 4 to 8 processor systems
- 3X to 6X speedup possible on high end server systems (IBM, HP, SGI ..)

Usage Guidelines: Sparse



- **Resource requirements**

- Total factorization time depends on model geometry and element type
 - Shell models best
 - Bulky 3-D models with higher order elements more expensive
- System requirements
 - 1 Gbyte per million dofs
 - 10 Gbyte disk per million dofs
- Eventually runs out of resource
 - 10 million dofs = 100 Gbyte file
 - 100 Gbytes X 3 = 300 Gbytes I/O
 - 300 Gbytes @ 30 Mbytes/sec = approx. 10,000 seconds I/O wait time

Usage Guidelines: PCG



- **Capabilities**

- Runs in-core, supports out-of-core (you don't need to do this)
- Parallel matrix/vector multiply achieves 2X on 4 to 8 processor system
- Memory saving element-by-element technology for solid92 (and solid95 beta in 6.1)

Usage Guidelines:PCG



- **Resource requirements**
 - 1 Gbyte per million dofs
 - Memory grows automatically for large problems
 - I/O requirement is minimal
 - Convergence is best for meshes with good aspect ratios
 - 3-D cube elements converge better than thin shells or high aspect solids
 - Over 500k dofs shows best performance compared to sparse

Usage Guidelines: Substructuring



- Eqsolv,spar in generation pass
 - Requires pcg or sparse in expansion pass
- Use pass uses sparse solver by default
 - May fail in symbolic assembly (try asso,,front)
- Pcg or sparse in expansion pass
 - Avoids large tri files

This is Beta feature only in 6.1, no unsymmetric, no damping

Performance Summary



- **Where to look**
 - PCG solver; file.PCS
 - Sparse solver; output file
 - Add Bcsopt ,,, ,,, -5 (undocu. Option)
- **What to look for**
 - Degrees of freedom
 - Memory usage
 - Total iterations (iterative only)

Usage Guidelines



- Tuning sparse solver performance
 - Bcsopt command (undocumented)
 - Optimal I/O for largest jobs
 - In-core for large memory systems and small to medium jobs ($< 250,000$ dofs)
 - Use parallel processing

User Control of Sparse Solver Options



Sparse solver control using undocumented command:

bcsopt, ropt, mopt, msiz ,,, dbg

mmd
metis
sgi
wave

Set equation
reordering
method

forc
limit

Force or limit
solver memory
space in Mbytes

nnnn - Mbytes
up to 2048

-5

Print
performance
stats

Solvers and Modal Analyses



- **Modal analyses most demanding in ANSYS**
 - Block Lanczos is most robust
 - Requires all of sparse solver resources plus additional space for eigenvectors
 - Requires multiple solves during Lanczos iterations
 - Subspace good for very large jobs and few eigenvalues
 - Uses PCG solver
 - Or uses the frontal solver
 - Not as robust as block Lanczos

Some Solver Examples



- Some benchmarks 5.7 vs 6.0
- Typical large sparse solver jobs
- Sparse solver memory problem
- PCG solver example
- AMG solver examples

Benchmark study; Static analysis



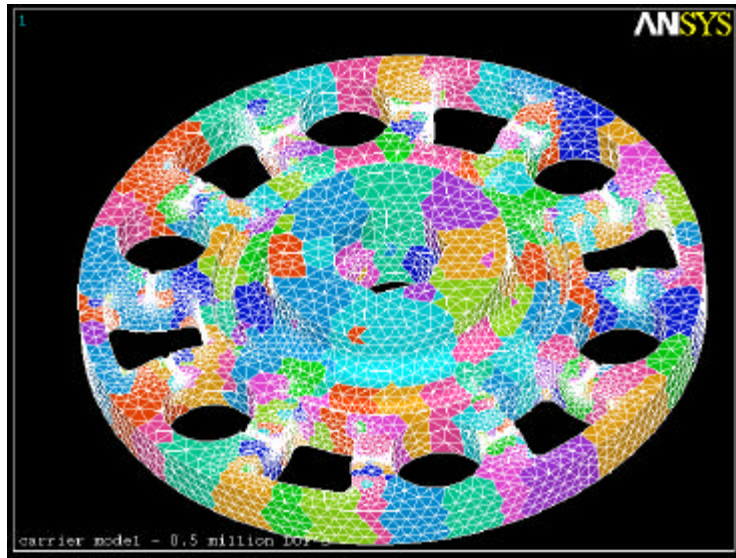
	<i>DOF</i>	<i>Total Solution Time</i>		<i>Peak Memory</i>	
		5.7	6	5.7	6
Sparse Solver					
Beam	110838	320	289	58	124
Car	421677	1149	789	1124	940
Joint	502851	2123	1146	480	312
Carrier2	502851	3113	1893	1115	1115
Carrier1	980484	4662	2736	1665	1196
RailCar	1470915	4257	3531	1084	1084
Engine	1676660	x	7967	x	1466
Assembly	3388179	x	18091	x	2873
PCG					
Car	421677	4215	4215	268	269
Joint	502851	1014	1014	294	294
Carrier2	502851	763	763	349	349
Carrier1	980484	1167	1147	677	677
RailCar	1470915	7488	7488	862	862
Engine	1676660	13770	13770	1235	1235
Assembly	3388179	x	x	x	x

Benchmark study:ModalAnalysis



	<i>DOF</i>	<i>Total Solution Time</i>		<i>Peak Memory</i>	
		5.7	6	5.7	6
	Sparse Solver				
Beam	110838	320	289	58	124
Car	421677	1149	789	1124	940
Joint	502851	2123	1146	480	312
Carrier2	502851	3113	1893	1115	1115

Sparse Solver Memory Usage Example 1



2 Million DOF Sparse solver job
SGI O2000 16 CPU system

MultiSolution: Sparse Assembly Option Call No. 1

ANSYS largest memory block available	10268444 :	9.79 Mbytes
ANSYS memory in use	1323917280 :	1262.59 Mbytes

End of PcgEnd

ANSYS largest memory block available	588214172 :	560.96 Mbytes
ANSYS memory in use	256482560 :	244.60 Mbytes
Total Time (sec) for Sparse Assembly	63.53 cpu	69.02 wall

Heap space available at start of BCSSL4: nHeap= 75619667 D.P. words 576.93 Mbytes

577 Mbytes available for sparse solver

Sparse Solver Memory Usage Example 1 (cont.)



Carrier 2M dof Model

ANSYS 6.0 memory allocation

```
SPARSE MATRIX DIRECT SOLVER.  
Number of equations =2090946,    Maximum wavefront =    275  
  
Heap space available at start of bcs_mem0: nHeap=  
61665329 D.P. words    470.47 Mbytes  
  
Estimated work space needed for solver: min_siz=  
256932078 D.P. words    1960.24 Mbytes  
  
Start_siz Work space needed for solver: start_siz=  
110399416 D.P. words    842.28 Mbytes  
  
Heap space setting at start of bcs_mem0: nHeap=  
110399416 D.P. words    842.28 Mbytes  
Initial BCS workspace memory =    110399416 D.P. words    842.28 Mbytes  
  
Total Reordering Time (cpu,wall) =    537.670    542.897  
  
Increasing memory request for BCS work to    67802738 D.P. words    517.29 Mbytes  
Initial BCS workspace is sufficient  
Memory available for solver =    842.28 MB  
Memory required for in-core =    0.00 MB  
Optimal memory required for out-of-core =    517.29 MB  
Minimum memory required for out-of-core =    162.39 MB
```

Initial memory increased
to 800 Mbytes

800 Mbytes exceeds
Optimal I/O setting

Initial guess easily runs in optimal I/O mode

Sparse Solver Memory Usage Example 1 (cont.)



Carrier2 2M dof Model

```
number of equations           =      2090946
no. of nonzeros in lower triangle of a =      84553633
no. of nonzeros in the factor l =     2434337580
maximum order of a front matrix =           9645
maximum size of a front matrix  =      46517835
no. of floating point ops for factor =     7.4048E+12

time (cpu & wall) for structure input =      193.810000      223.923436
time (cpu & wall) for ordering         =      456.970000      461.192527
time (cpu & wall) for symbolic factor  =           7.400000           7.471412
time (cpu & wall) for value input       =      287.240000      384.408332
time (cpu & wall) for numeric factor    =     12671.900000     13367.557193
computational rate (mflops) for factor =      584.351978      553.941885
time (cpu & wall) for numeric solve     =      765.760000     1411.694416
computational rate (mflops) for solve   =      12.729582        6.905039
```

```
i/o statistics:  unit number      length      amount
                  -----
                    20.      138591505.      288939194.
                    25.       9310592.       32587072.
                     9.      2434337580.      7894888171.
                    11.      169107266.      507331541.
```

Freeing BCS workspace

Sparse Matrix Solver CP Time (sec) = 14468.280

Sparse Matrix Solver ELAPSED Time (sec) = 15982.407

2.1M Dofs

84M Nzeros in K (40/1)

2.4B Nzeros in L (1142/29)

7.4 Trillion F.P. ops

Factored Matrix file LN09

2.4 Billion D.P words, 18 Gbytes
59 Gbytes transferred

File LN32 not used

Elapsed time close to CPU time (4.5 Hours)
Good processor utilization, reasonable I/O performance

Engine Block Analysis

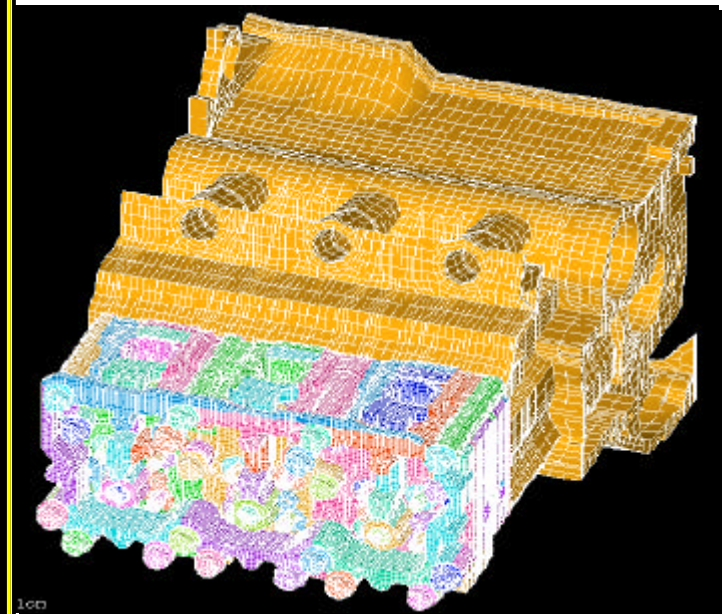
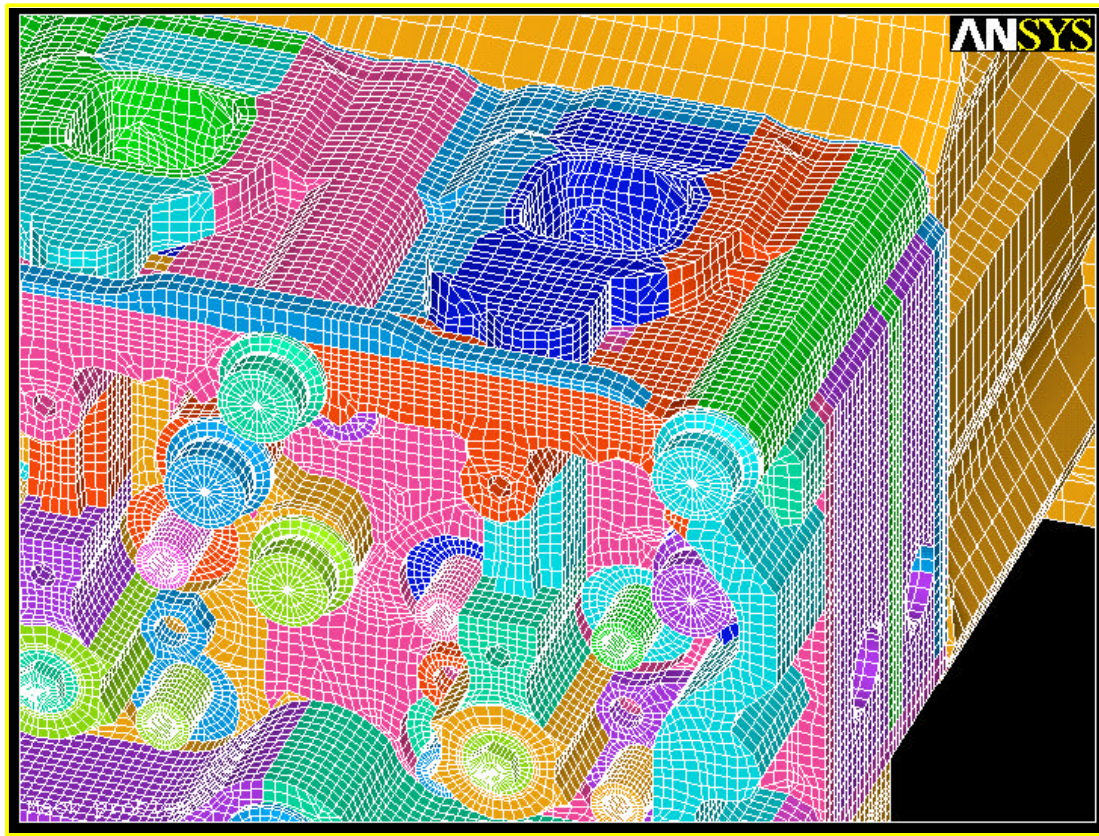


410,977 Solid45 Elements

16,304 Combin40 Elements

1,698,525 Equations

20,299 Multi-Point CEs



Engine Block Analysis



Sparse Solver Interface Statistics

Sparse CE interface Matrix	dim	coefs	mxcolmlth
-----	*****	*****	*****
Original A22	1698525	55419678	209
Constraints G	20299	58147	6
H = G*A11 + A12T	20299	860830	99
HGT	1698525	865275	381
Modified A22	1698525	58304862	404

of columns modified by direct elimination of CEs:132849

Over 20,000 CEs processed with minimal additional memory required

Memory available for solver = 547.22 MB
Memory required for in-core = 9417.10 MB
Optimal memory required for out-of-core = 527.29 MB
Minimum memory required for out-of-core = 127.25 MB

Memory available is sufficient to run in Optimal I/O mode

Engine Block Analysis



Sparse Solver Performance Summary

SGI O2000 16-300Mhz Processors, 3 CPU run

```
time (cpu & wall) for structure input = 162.05    172.82
time (cpu & wall) for ordering        = 340.37    342.63
time (cpu & wall) for symbolic factor = 7.93      7.96
time (cpu & wall) for value input     = 225.89    267.12
time (cpu & wall) for numeric factor  = 4812.04   5086.30
computational rate (mflops) for factor = 592.55    560.60
time (cpu & wall) for numeric solve   = 365.90    663.77
computational rate (mflops) for solve = 12.54      6.91
```

I/O always shows
up in solve

```
i/o statistics:  unit number      length      amount
                  -----
                    20      91464700    192879558
                    25      5319910     18619685
                     9    1145424928    3816657199
                    11    108680690     615455923
```

Good sustained rate on factorization – nearly 600 mflops

Sparse Solver Example 2



What can go wrong

Customer example: excessive elapsed time
High Performance HP 2 CPU desktop system

Release 6.0	UP20010919	HPPA 8000-64
Maximum Scratch Memory Used	= 252053628 Words	961.508 MB
CP Time (sec) =	6323.090	Time = 23:36:41
Elapsed Time (sec) =	27575.000	Date = 01/10/2002

Sparse Solver Example 2 (cont.)



FEM model of large radiator
650k Degrees of Freedom

68,000 Solid95 Elements
2089 Surf154 Elements
3400 Constraint Equations

Initial memory setting –m 1000 –db 300

Sparse Solver Example 2 (cont.)



```
MultiSolution: Sparse Assembly Option .... Call No. 1
  ANSYS largest memory block available      73741452 :    70.33 Mbytes
  ANSYS memory in use                      612110368 :   583.75 Mbytes
```

584 Mbytes in use
during sparse Assembly

```
Sparse Solver Interface Adding CEs.... Call No. 1
  ANSYS largest memory block available      73741164 :    70.33 Mbytes
  ANSYS memory in use                      612110656 :   583.75 Mbytes
```

```
Sparse CE interface Matrix    dim      coefs  mxcolmlth
-----
      Original A22    648234  41415993      461
      Constraints G      3471    23222        8
      H = G*A11 + A12T    3471   409194      219
      HGT      648234    781339      668
```

The initial memory allocation (-m) has been exceeded.
Supplemental memory allocations are being used.

Needs more memory
to process CEs

```
No. of columns modified by direct elimination of CEs:    42558
      Modified A22    648234  43974225      692
  ANSYS largest memory block available    288465472 :   275.10 Mbytes
  ANSYS memory in use                    179570288 :   171.25 Mbytes
Total Time (sec) for processing CEs    38.33 cpu    61.73 wall
End of PcgEnd
  ANSYS largest memory block available    575083952 :   548.44 Mbytes
  ANSYS memory in use                    133219536 :   127.05 Mbytes
Total Time (sec) for Sparse Assembly    38.36 cpu    61.77 wall
```

548 Mbytes available
after sparse Assembly

Sparse Solver Example 2 (cont)



Minimum core memory run: 650k dofs

Memory available for solver = 488.21 MB
Memory required for in-core = 7348.80 MB
Optimal memory required for out-of-core = 651.66 MB
Minimum memory required for out-of-core = 63.18 MB

488 Mbytes available is
less than optimal I/O memory

time (cpu & wall) for structure input	=	40.130000	62.959089
time (cpu & wall) for ordering	=	269.940000	296.114490
time (cpu & wall) for symbolic factor	=	6.780000	8.303449
time (cpu & wall) for value input	=	127.230000	624.087842
time (cpu & wall) for numeric factor	=	5312.130000	25199.576871
computational rate (mflops) for factor	=	740.325416	156.062337
condition number estimate	=	0.0000D+00	
time (cpu & wall) for numeric solve	=	117.400000	890.047902
computational rate (mflops) for solve	=	28.598027	3.772166

i/o statistics:	unit number	length	amount
	-----	-----	-----
	20.	77728422.	173599480.
	25.	3414388.	11950358.
	9.	838554505.	2753998119.
	11.	84582582.	723248228.
	32.	77134410.	11000063203.

Factored Matrix file LN09
838M D.P words, 6.4 Gbytes
21 Gbytes transferred

Sparse Matrix Solver CP Time (sec) = 5956.170
Sparse Matrix Solver ELAPSED Time (sec) = 27177.617

*Elapsed time 5X
larger than CPU time!*

Large front spillover file I/O is culprit
77M D.P. words, 110 Billion transferred!
Over $\frac{3}{4}$ of a Terabyte transferred!!!

Sparse Solver Example 2 (cont)



Optimal out-of-core memory run: 650k dofs

Memory available for solver = 660.21 MB
Memory required for in-core = 7348.80 MB
Optimal memory required for out-of-core = 651.66 MB
Minimum memory required for out-of-core = 63.18 MB

660 Mbytes available is
achieves optimal I/O memory

time (cpu & wall) for structure input	=	40.170000	62.870488
time (cpu & wall) for ordering	=	270.470000	294.560051
time (cpu & wall) for symbolic factor	=	6.770000	8.156075
time (cpu & wall) for value input	=	116.300000	360.649415
time (cpu & wall) for numeric factor	=	4773.720000	3418.024528
computational rate (mflops) for factor	=	823.823853	1150.578169
condition number estimate	=	0.0000D+00	
time (cpu & wall) for numeric solve	=	115.450000	880.488530
computational rate (mflops) for solve	=	29.081060	3.813120

1 Gflop sustained

i/o statistics:	unit number	length	amount
	-----	-----	-----

20.	77728422.	173599480.
25.	3414388	11950358.
9.	838554505.	2674553251.
11.	80694876	470400286.

Factored Matrix file LN09
838M D.P words, 6.4 Gbytes
21 Gbytes transferred

Sparse Matrix Solver CP Time (sec) = 5405.520
Sparse Matrix Solver ELAPSED Time (sec) = 5122.035

File LN32 not used

*Elapsed time 5X faster
than minimum memory run*

Sparse Solver NT system Example



What can go wrong

Customer example: NT memory problems

Dell system, 2 P4 processors, 2 Gbytes memory

- default memory run failed
- -m 925 -db 100 failed before solver
- -m 1100 -db 100 interactive failed
- -m 1100 -db 100 batch mode worked

Why so memory sensitive???

Sparse Solver NT system example (cont)



FEM model of turbine blade

772k Degrees of Freedom

114,000 Solid45 Elements

4662 Solid 95 Elements

76173 Solid 92 Elements

18118 Surf154 Elements

3400 Constraint Equations

Lots of CEs used to impose cyclic symmetry conditions

Sparse Solver NT system (cont.)



NT system run, 770k dofs turbine blade

```
MultiSolution: Sparse Assembly Option .... Call No. 1
  ANSYS largest memory block available  288061264 :   274.72 Mbytes
  ANSYS memory in use                   562923008 :   536.85 Mbytes
```

537 Mbytes in use
Before CEs

```
Sparse Solver Interface Adding CEs.... Call No. 1
  ANSYS largest memory block available  288061024 :   274.72 Mbytes
  ANSYS memory in use                   562923248 :   536.85 Mbytes
```

Sparse CE interface Matrix	dim	coefs	mxcolmlth
-----	*****	*****	*****
Original A22	772125	28566123	0
Constraints G	16533	71706	0
H = G*A11 + A12T	16533	895685	0
HGT	772125	8364601	0

Needs more memory
to process CEs

The initial memory allocation (-m) has been exceeded.
Supplemental memory allocations are being used.

No. of columns modified by direct elimination of CEs: 51678

Sparse CE interface Matrix	dim	coefs	mxcolmlth
-----	*****	*****	*****
Modified A22	772125	61587249	0

```
ANSYS largest memory block available  4971036 :    4.74 Mbytes
  ANSYS memory in use                   1502114112 :  1432.53 Mbytes
```

```
ANSYS largest memory block available  804449536 :   767.18 Mbytes
  ANSYS memory in use                   185689952 :   177.09 Mbytes
Total Time (sec) for Sparse Assembly   79.95 cpu   80.48 wall
```

1432 Mbytes in use
after CEs

1400 Mbytes is well over initial allocation !

Sparse Solver NT example (cont)



Optimal I/O run on fast NT system: 770k dofs

Using opt out of core memory setting

Initial BCS workspace is sufficient

Memory available for solver = 719.93 MB
Memory required for in-core = 6944.94 MB
Optimal memory required for out-of-core = 623.68 MB
Minimum memory required for out-of-core = 77.61 MB

720 Mbytes available
achieves optimal I/O memory

time (cpu & wall) for structure input	=	25.484000	25.643644
time (cpu & wall) for ordering	=	108.000000	108.698163
time (cpu & wall) for symbolic factor	=	4.531000	4.555646
time (cpu & wall) for value input	=	217.094000	218.496403
time (cpu & wall) for numeric factor	=	2224.359000	2238.762857
computational rate (mflops) for factor	=	1335.468214	1326.876016
condition number estimate	=	0.0000D+00	
time (cpu & wall) for numeric solve	=	824.610000	829.907434
computational rate (mflops) for solve	=	3.759268	3.735272

1.3 Gflops sustained

i/o statistics:	unit number	length	amount
	-----	-----	-----

20.	55724809.	118615367.
25.	3780444	13231554.
9.	774037991.	2451597713.

Factored Matrix file LN09
774M D.P words, 5.7 Gbytes
18 Gbytes transferred

Sparse Matrix Solver CP Time (sec) = 3432.969
Sparse Matrix Solver ELAPSED Time (sec) = 3455.119

File LN32 not used

Excellent performance once memory issue is resolved!!

Usage Guidelines: Substructuring



- Eqslv,spar in generation pass
 - Requires pcg or sparse in expansion pass
- Use pass uses sparse solver by default
 - May fail in symbolic assembly (try asso,,front)
- Pcg or sparse in expansion pass
 - Avoids large tri files

This is Beta feature only in 6.1, no unsymettric, no damping

Solving NT memory issues



- Try default memory management
- Maximize solver memory
 - Use larger db for prep and post only
 - Reduce db memory for solve
 - Run in batch mode
- Read output file memory messages
 - Leave room for supplemental memory allocations
 - Try bcsopt,,forc,msiz as a last resort

How to get Optimal I/O Memory



- Prior to 6.1
 - Increase `-m`, decrease `-db`
 - Force sparse memory with `bcsopt`
- Version 6.1
 - Automatic in most cases
 - Tuning possible using `bcsopt`
- WINTEL 32 bit limitations
 - Total process space 2Gbytes
 - Keep `db` space small to maximize sparse solver memory
 - Don't start `-m` too small for large jobs
 - Use `msave,on` for PCG solver

Sparse Solver Example 3



ANSYS 6.1 example – 2 Million DOF engine block

Start of BCS_MEM1: msglvl= 2

need_in=	0	D.P. words	0.00	Mbytes
need_opt=	221585885	D.P. words	1690.57	Mbytes
need_ooc=	20333932	D.P. words	155.14	Mbytes
nHold0=	202309239	D.P. words	1543.50	Mbytes
nHeap=	11789065	D.P. words	89.94	Mbytes
navail=	202309239	D.P. words	1543.50	Mbytes
mem_siz=	0	D.P. words	0.00	Mbytes

Sparse solver memory is just below optimal setting

Grow memory to optimal setting

Increasing memory request for BCS work to 221585885 D.P. words 1690.57 Mbytes

The initial memory allocation (-m) has been exceeded.
Supplemental memory allocations are being used.

After Realloc: pdHold= -1575830551 hHold0= 324 nHold= 221585885
Memory available for solver = 1690.57 MB
Memory required for in-core = 0.00 MB
Optimal memory required for out-of-core = 1690.57 MB
Minimum memory required for out-of-core = 155.14 MB

Sparse Solver Example 3 (cont.)



ANSYS 6.1 Engine Block example: SGI O2000 system

```
number of equations = 2149066
no. of nonzeros in lower triangle of a = 78007632
no. of nonzeros in the factor l = 2698281519.
maximum order of a front matrix = 20062
maximum size of a front matrix = 201251953
no. of floating point ops for factor = 1.9072E+13
no. of floating point ops for solve = 1.0804E+10
time (cpu & wall) for structure input = 181.640000 191.469832
time (cpu & wall) for ordering = 800.110000 807.598554
time (cpu & wall) for symbolic factor = 10.520000 10.572956
time (cpu & wall) for value input = 259.820000 345.327975
time (cpu & wall) for numeric factor = 30088.200000 31027.369107
computational rate (mflops) for factor = 633.883809 614.696745
time (cpu & wall) for numeric solve = 768.060000 1634.010750
computational rate (mflops) for solve = 14.066442 6.611873
```

2.1M Dofs
78M Nzeros in K (37/1)
2.7B Nzeros in L (1286/35)
19 Trillion F.P. ops

```
i/o statistics:  unit number      length      amount
                  -----      -
```

	20.	129721091.	272147055.
	25.	7964778.	27876723.
	9.	2698281519.	8406875085.
	11.	250835024.	1964282370.

Freeing BCS workspace

Dealloc ptr_Diag= 683102464

Sparse Matrix Solver CP Time (sec) = 32283.010

Sparse Matrix Solver ELAPSED Time (sec) = 34199.480

Factored Matrix file LN09
2.7 Billion D.P words, 20 Gbytes
63 Gbytes transferred

File LN32 not used

Elapsed time close to CPU time (10 Hours)

PCG Solver Example



- PCG memory grows dynamically in non-contiguous blocks
- Msave,on skips global assembly of stiffness matrix for SOLID 92, 95 elements.
- PCG solver can do largest problems in the least memory

PCG Solver Example (cont.)

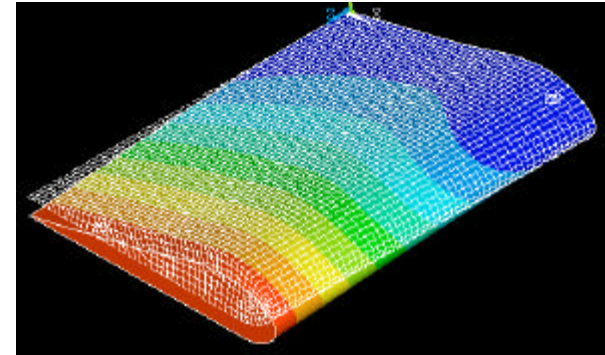


Wing job example, 500k dofs, SOLID45 elements

```
Degrees of Freedom: 477792
DOF Constraints: 4424
Elements: 144144
      Assembled: 144144
      Implicit: 0
Nodes: 159264
Number of Load Cases: 1

Nonzeros in Upper Triangular part of
      Global Stiffness Matrix : 18350496
Nonzeros in Preconditioner: 7017045
```

File.PCS output



```
Total Operation Count: 3.71503e+10
Total Iterations In PCG: 343
Average Iterations Per Load Case: 343
Input PCG Error Tolerance: 1e-06
Achieved PCG Error Tolerance: 9.90796e-07
```

Good convergence
(1000 or more is bad)

DETAILS OF SOLVER CP TIME(secs)	User	System
Assembly	23.9	3.6
Preconditioner Construction	8.7	1.8
Preconditioner Factoring	0.9	0
Preconditioned CG	273.9	0.3

```
Total PCG Solver CP Time: User: 320.9 secs: System: 9.9 secs
```

```
Estimate of Memory Usage In CG : 240.191 MB
```

```
Estimate of Disk Usage : 247.919 MB
```

```
CG Working Set Size with matrix outcore : 65.0977 MB
```

```
Multiply with A MFLOP Rate:168.24 MFlops
```

```
Solve With Precond MFLOP Rate:111.946 MFlops
```

Memory usage and disk I/O low

Mflops performance always
Lower than sparse solver

PCG Solver Example (cont.)



Wing job example, 228k dofs, SOLID95 elements

Msave,on

```
Degrees of Freedom: 228030
DOF Constraints: 3832
Elements: 16646
  Assembled: 0
  Implicit: 16646
```

```
Nonzeros in Upper Triangular part of
Global Stiffness Matrix : 0
Nonzeros in Preconditioner: 4412553
```

```
Total Operation Count: 1.06317e+10
Total Iterations In PCG: 488
```

```
*****
Total PCG Solver CP Time: User: 809.6 secs:
*****
Estimate of Memory Usage In CG : 30.6945 MB
Estimate of Disk Usage   : 36.5936 MB
```

```
*** Implicit Matrix Multiplication Activated
*****
Multiply with A MFLOP Rate:0 MFlops
Solve With Precond MFLOP Rate:81.7201 MFlops
*****
```

Default

```
Degrees of Freedom: 228030
DOF Constraints: 3832
Elements: 16646
  Assembled: 16646
  Implicit: 0
```

```
Nonzeros in Upper Triangular part of
Global Stiffness Matrix : 18243210
Nonzeros in Preconditioner: 4412553
```

```
Total Operation Count: 4.60199e+10
Total Iterations In PCG: 488
```

```
*****
Total PCG Solver CP Time: User: 850.2 secs:
*****
Estimate of Memory Usage In CG : 208.261 MB
Estimate of Disk Usage   : 215.985 MB
```

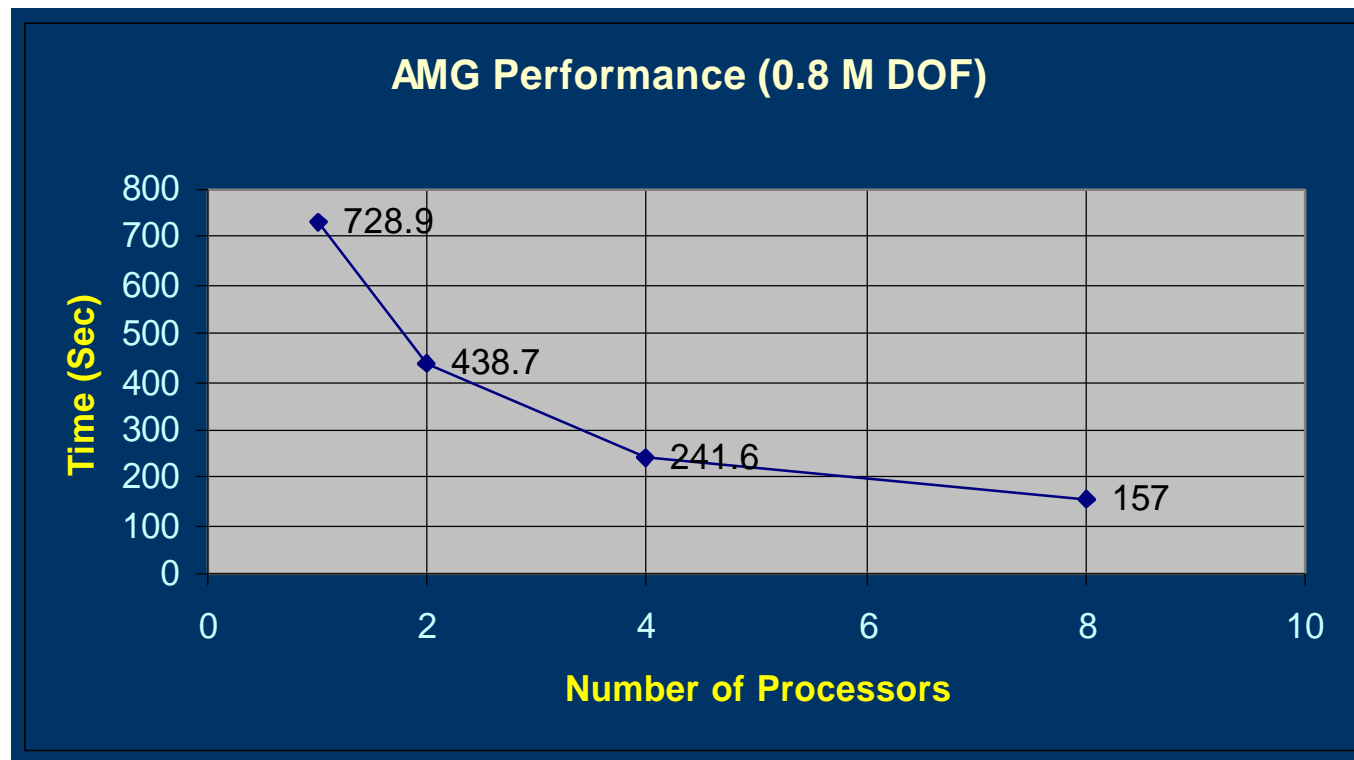
```
*****
Multiply with A MFLOP Rate:62.3031 MFlops
Solve With Precond MFLOP Rate:53.5653 MFlops
*****
```

*Msave,on saves 170 Mbytes out of 200 Mbytes
Solve time is comparable to assembled run
Works only for SOLID 92s and SOLID95s in 6.1*

AMG Performance



Solver time (sec) vs number of processors



AMG vs PowerSolver



Advantages:

- Insensitive to matrix ill-conditioning.
Performance doesn't deteriorate for high aspect ratio elements, rigid links, etc
- 5x faster than the PowerSolver for difficult problems on a single processor
- Scalable up to 8 processors (shared- memory only), 5 times faster with 8 processors

AMG vs PowerSolver



Disadvantages:

- 30% more memory required than PowerSolver
- 20% slower than PowerSolver for well conditioned problems on a single processor
- Doesn't work for Distributed-Memory architecture (neither does PowerSolver).
- Scalability is limited by memory bandwidth (so is PowerSolver)

AMG vs Sparse Solver



ANSYS 6.1 example – 2 Million DOF engine block

AMG ITERATIVE SOLVER:

Number of equations = 2157241

Number of processors used = 8

Reading parameters from file amg_params.dat

anis_hard=4

anis_hard 4

hard=1

hard 1

end reading parameters

AMG parameters tuned for
Ill-conditioned problem

AMG NO.OF ITER = 102 ACHIEVED RESIDUAL NORM = 0.90170E-05

AMG ITERATIVE SOLVER ELAPSED TIME = 1758.000

Sparse Matrix Solver CP Time (sec) = 32283.010

Sparse Matrix Solver ELAPSED Time (sec) = 34199.480

AMG 19 times faster than sparse in this example

Comparative Performance may Vary



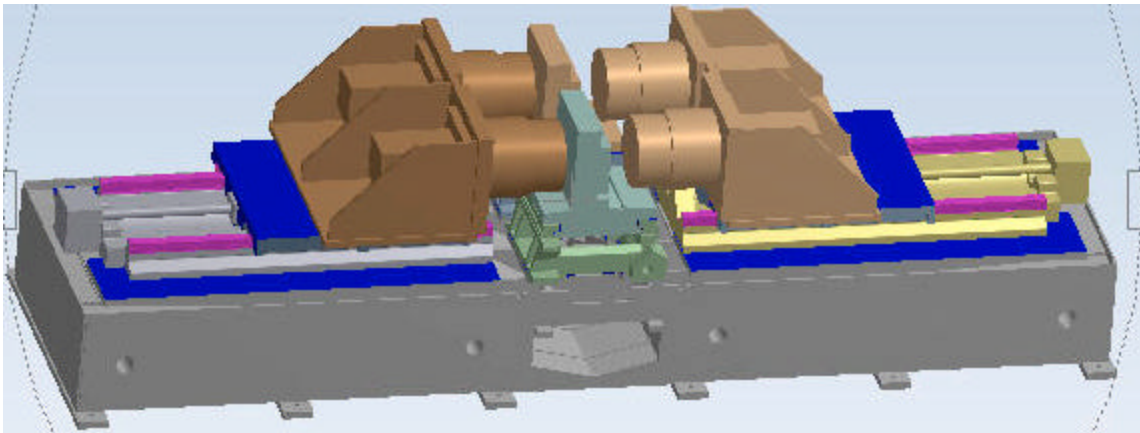
But,...

Your results may vary...

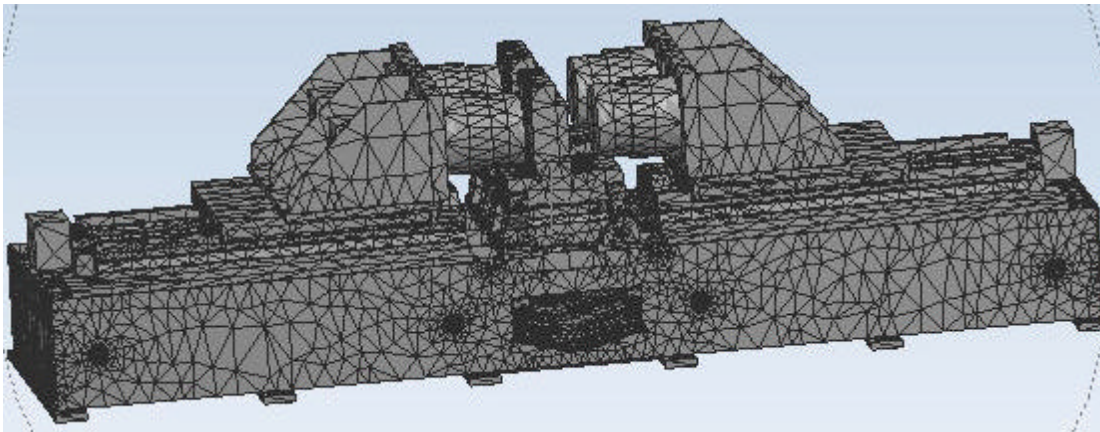
Large Industrial Example



Linear Static Analysis with Nonlinear Contact



ANSYS DesignSpace
Detailed Solid Model



Finite Element Model
119,000 Elements
590,000 DOFs

Large Industrial Example



Linear Static Analysis with Nonlinear Contact

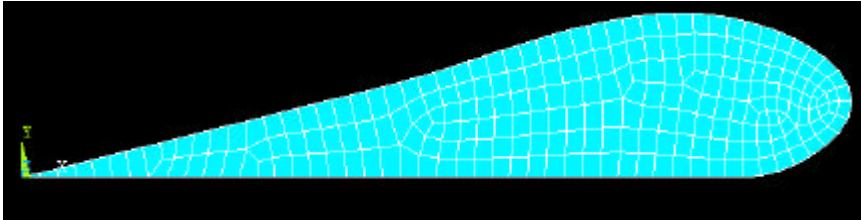
SGI O2000 16 300Mhz Processors, 16 Gbytes

Method	Memory Mbytes	Iter 10^{-6}	Solver Elapsed Time (sec)			
			NP=1	NP=2	NP=3	NP=4
PCG	300	5301	8679	7745	6636	6909
AMG	722	200	5265	3831	2638	1884
SPAR	290		881			

AMG shows superior convergence and scaling for this problem

BUT...Sparse Direct solver best for this problem

Wing Example Job



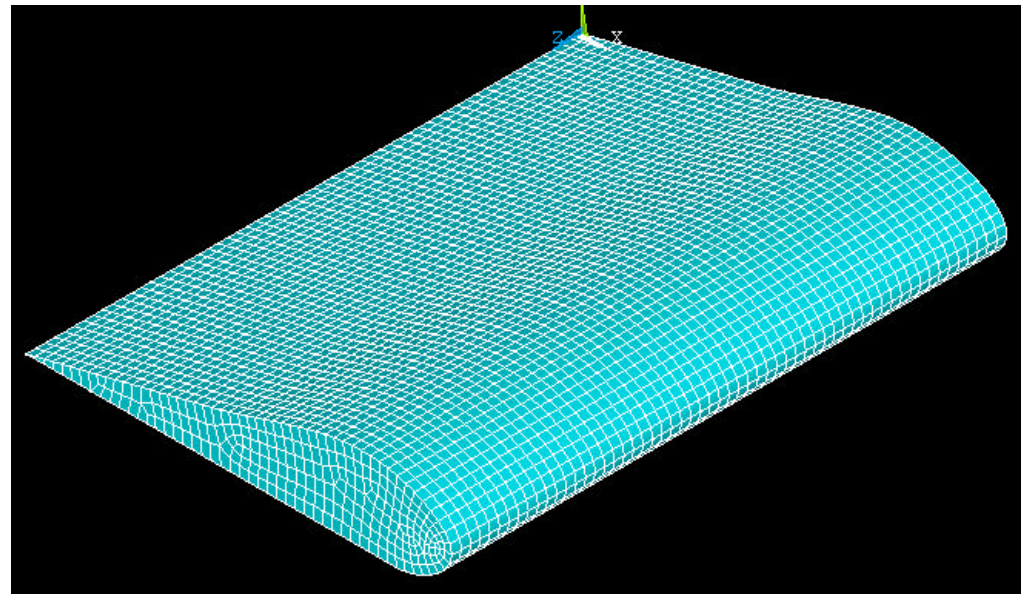
2-D mesh

282 nodes, 233 elements, 646 DOFs

-dofs 50

Extrude 2-D mesh to
obtain 50,000 Dofs

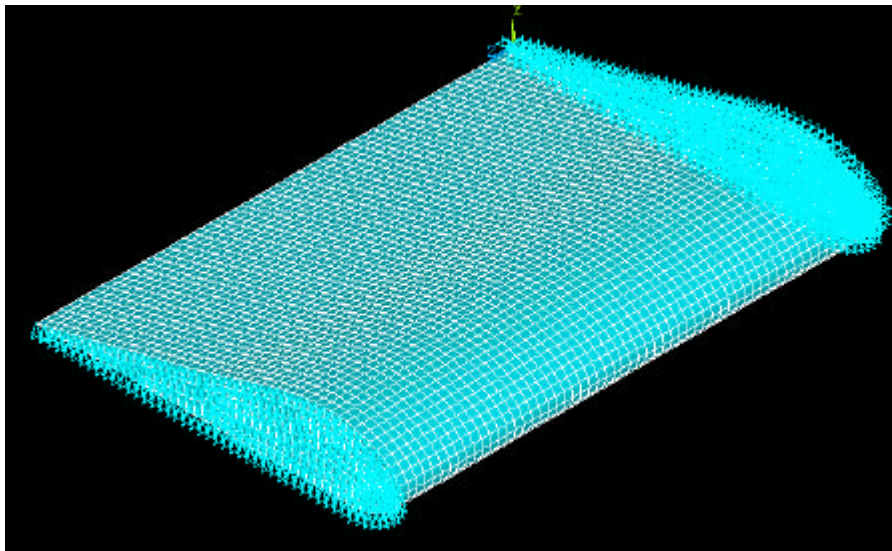
Elements sized to
maintain nice aspect
ratios



Wing Static Analyses



stype pcg, frontal, spar



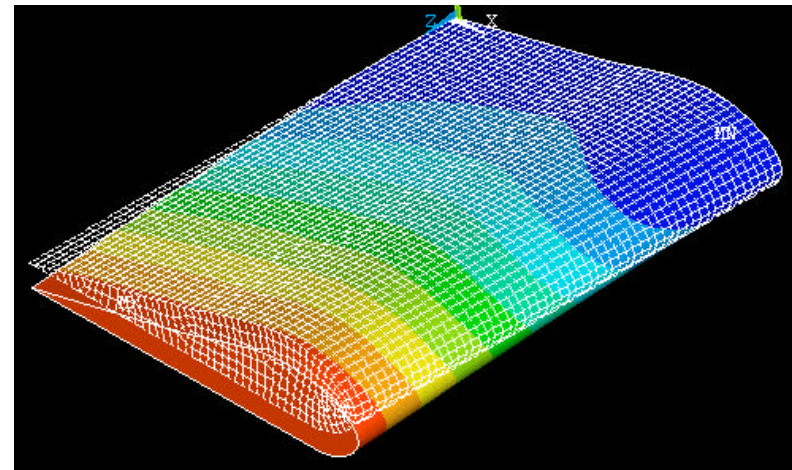
Fixed B.C.s at $z=0.0$

small negative y displacement at
opposite end

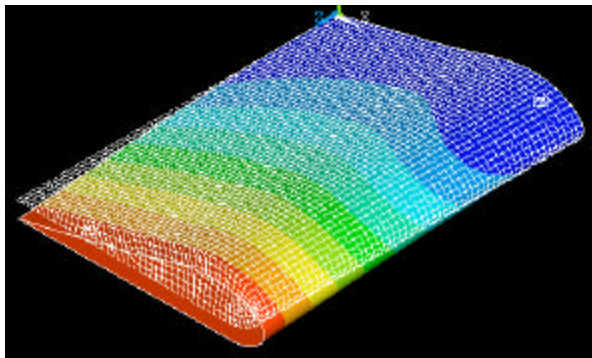
PowerSolver (pcg)

Frontal direct solver (frontal)

Sparse direct solver (spar)



Sparse Solvers Comparison

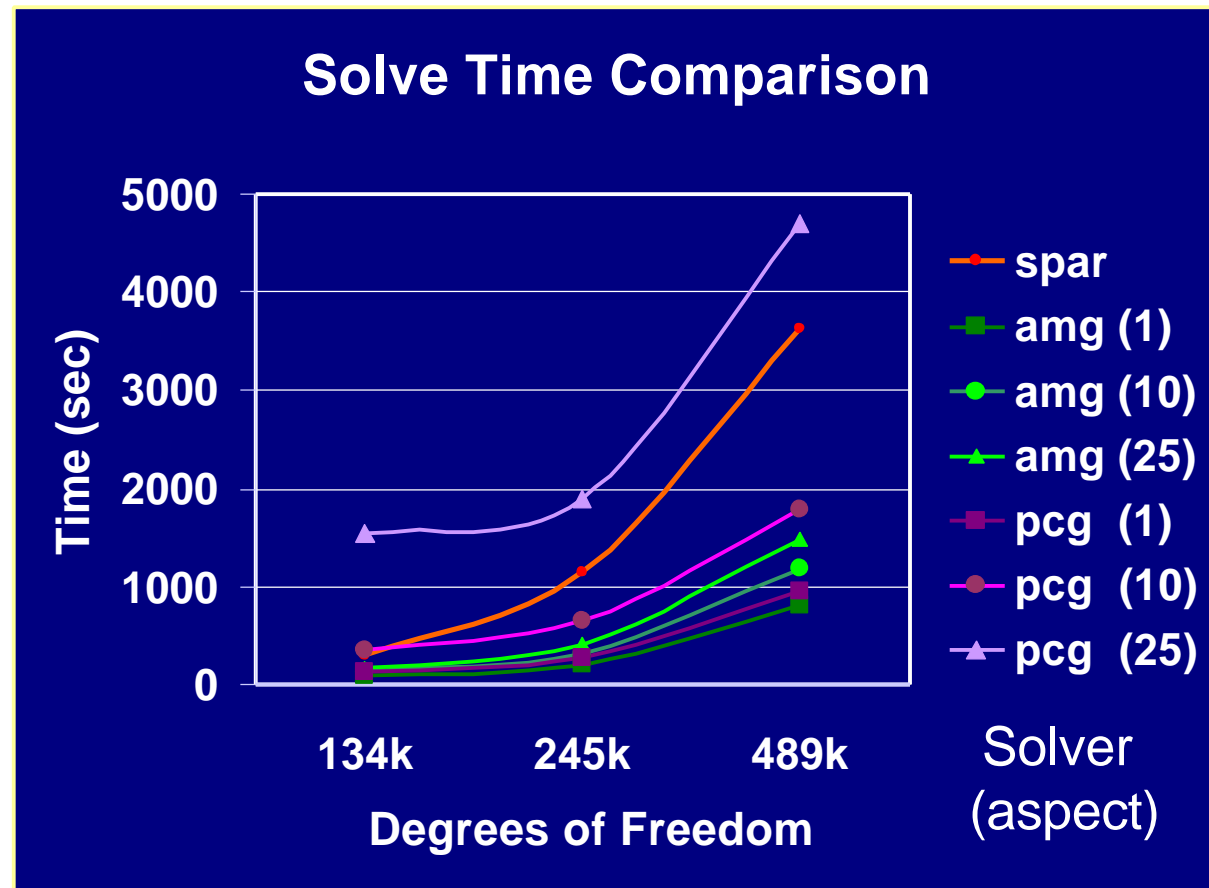


Static Analysis

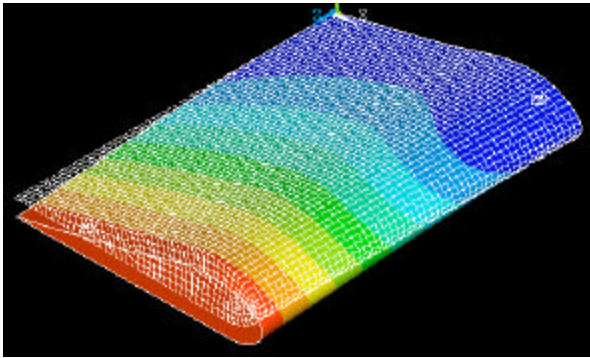
HP L-Class

Four 550 Mhz CPUs

4 Gbytes Memory



Sparse Solvers Comparison

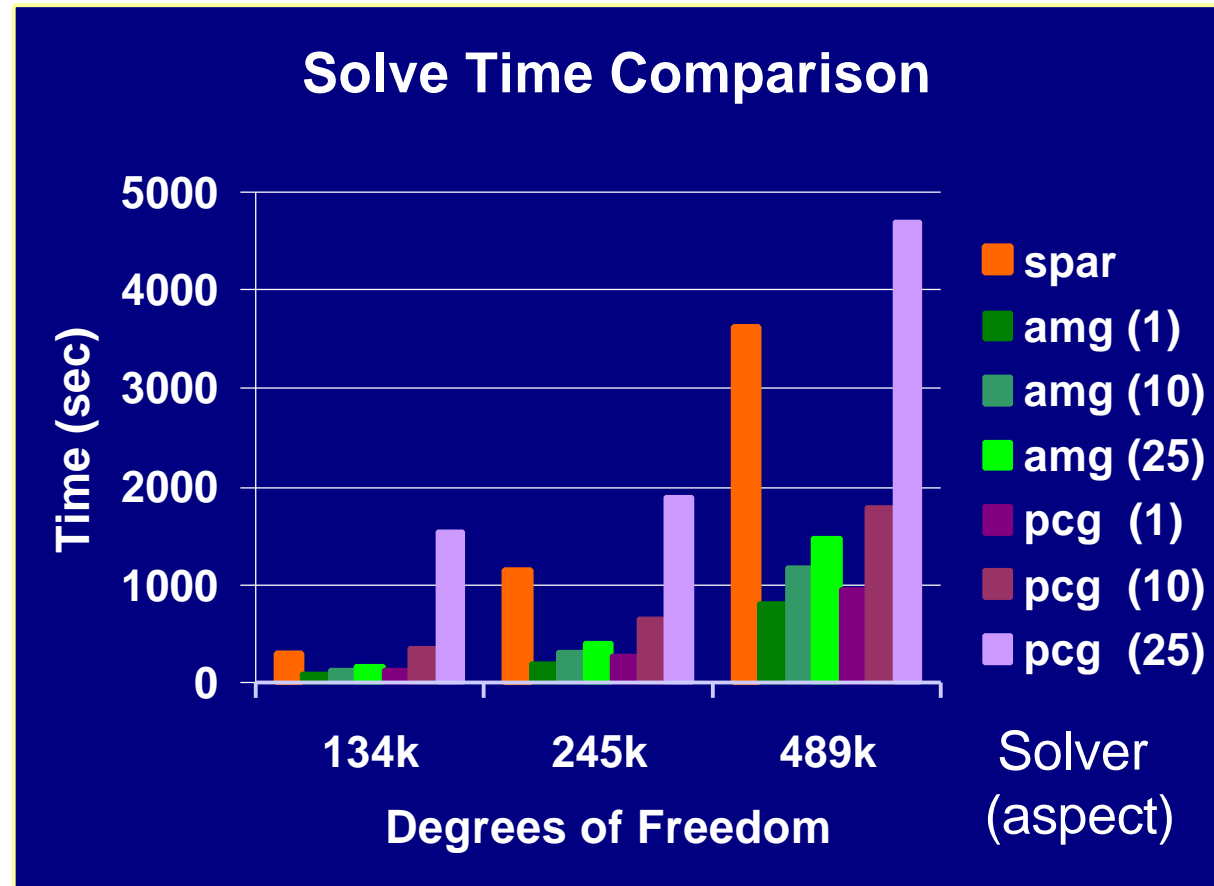


Static Analysis

HP L-Class

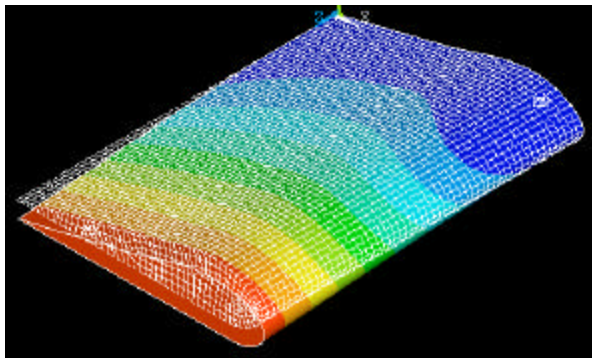
Four 550 Mhz CPUs

4 Gbytes Memory



Increasing aspect ratio makes matrices Ill-conditioned

Sparse Solvers Comparison

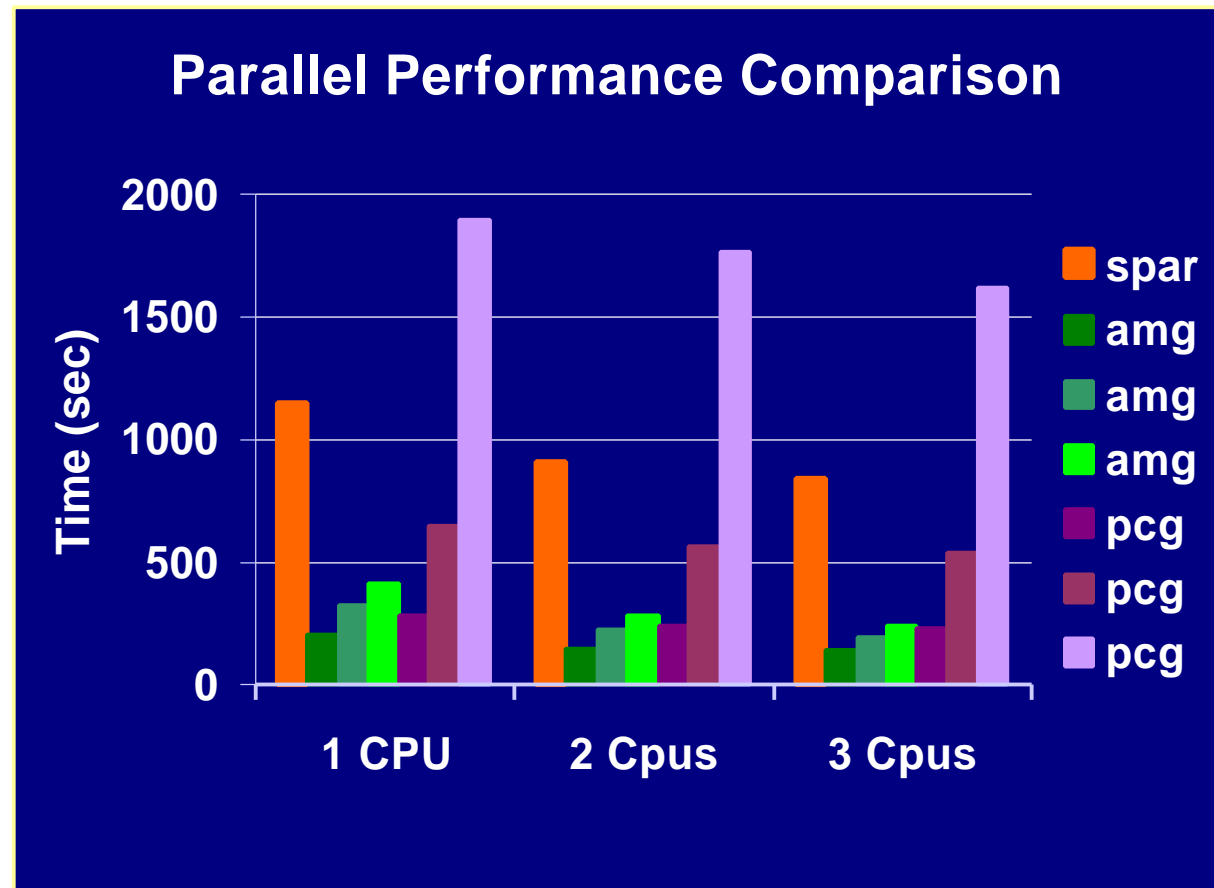


Static Analysis

HP L-Class

Four 550 Mhz CPUs

4 Gbytes Memory



Summary



- ANSYS has industry leading solver technology to support robust and comprehensive simulation capability
- Attention to solver capabilities and performance characteristics will extend analysis capabilities
- Future improvements will include increasing parallel processing capabilities and new breakthrough solver technologies