

Optimizing NX Nastran Performance

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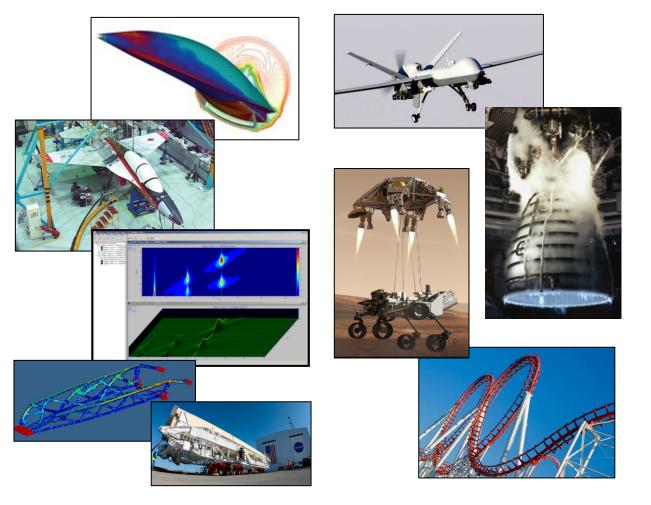
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Outline

What are Major Factors that Control Nastran Performance?

I/O, I/O and I/O

Understanding Nastran Files

- LP vs. ILP versions of Nastran
- Using .f04 file to understand performance

Effective Use on an HPC Cluster for NX Nastran

- Controlling amount of I/O Getting fast I/O
- Direct vs. Iterative solutions

Overview of Parallel Processing

• SMP, DMP, etc.

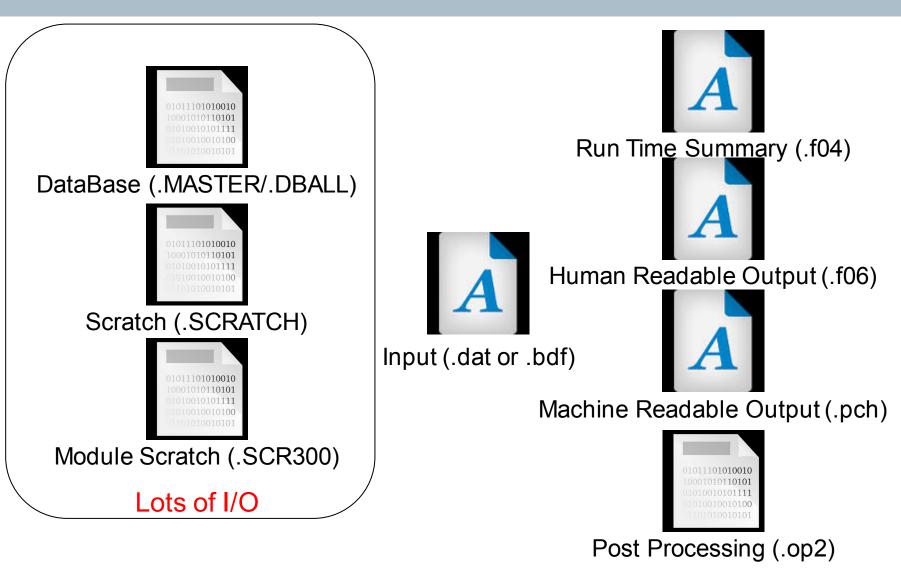
Goal is to provide you with tools to get best NX Nastran performance

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NX Nastran Performance by I/O, I/O, I/O

- To a large degree NXN performance governed by I/O speed to DBALL, SCRATCH and SCR300 files
- No matter what else you do if you don't have fast I/O for SCRATCH/SCR300 you don't have good performance



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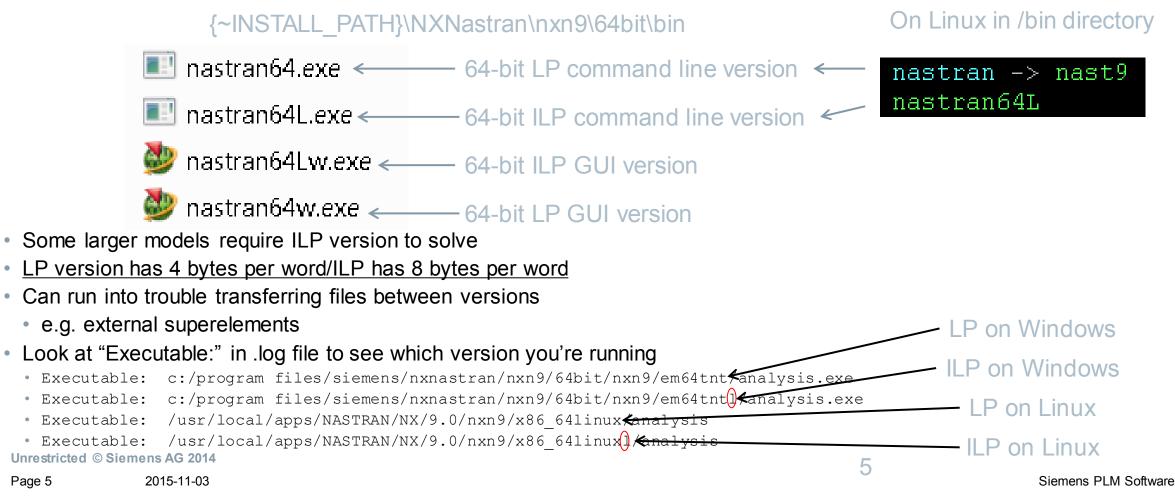
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Understanding LP/ILP Versions of NXN

All versions of NX Nastran come in 2 flavors

- LP uses 4 byte integers and addresses up to 8 GBytes of RAM
- ILP uses 8 byte integers and addresses large amount of RAM





To Understand Nastran Performance Need to Understand .f04 file!

To understand performance of any program we run a "profiler"

The .f04 file is Nastran's profiler output (effectively a DMAP line profiler)

Contains information on overall memory and disk usage as well as a step by step summary of every line of DMAP code that's executed:

Day_Time E	lapsed I/O_Mb	Del_Mb	CPU_Sec	Del_CPU	SubDMAP I	ine (S)	SubDMA	P/Module			
16:24:56	1:15 3845.0	5.0	70.1	0.0	SEMG 1	23 E	MG	BEGN			
*8** Module	DMAP Matrix	Cols	Rows F T	NzWds	Density	BlockT	StrL	NbrStr	BndAvg	BndMax	NulCol
EMG	123 KELM	5479	300 2 1	300 9	0.15904E-01	25	35	42490	292	300	0 *8**
EMG	123 MELM	5319	78 2 1	12 1	.53268E-01	3	0	63588	77	78	10 *8**
16:25:25	1:44 7685.0	2.0	93.4	0.0	XREAD 2	51 R	EAD	BEGN			
*** USER IN	FORMATION MESSAGE 41	57 (DFMSYN)									
PARAMETI	ERS FOR SPARSE DECOM	POSITION OF	DATA BLOCK	MXX (TYPE=RSP)	FOLLOW					
	MATRIX SIZ	E = 3151	6 ROWS	NUME	BER OF NONZE	ROES =	1113	7293 TERMS			
N	JMBER OF ZERO COLUMN	s =	0 NUM	BER OF ZERC	DIAGONAL 1	ERMS =		0			
	CPU TIME ESTIMAT	E = 62	SEC	I/C	TIME ESTIM	ATE =	0	SEC			
MINIM	JM MEMORY REQUIREMEN	т= 3499	K WORDS	ME	MORY AVAILA	BLE = 14	07554	K WORDS			
MEMORY I	REQR'D TO AVOID SPIL	L = 10636	K WORDS	MEMORY	USED BY BE	ND =	8311	K WORDS			
EST. IN	TEGER WORDS IN FACTO	r = 111	38 K WORDS	EST.	NONZERO TE	RMS =	1114	0 K TERMS			
ESTIMATI	ED MAXIMUM FRONT SIZ	E = 3141	TERMS		RANK OF UPD	ATE =	128				
16:25:25	1:44 7921.0	236.0	93.9	0.5	SPDC BGN	TE=62					
16:25:28	1:47 8155.0	234.0	97.0	3.1	SPDC END						
*** USER IN	FORMATION MESSAGE 64	39 (DFMSA)									
ACTUAL N	MEMORY AND DISK SPAC	E REQUIREME	NTS FOR SPARS	SE SYM. DEC	COMPOSITION						
SPAL	RSE DECOMP MEMORY US	ED = 1063	6 K WORDS	MAX	IMUM FRONT	SIZE =	3141	TERMS			
п	NTEGER WORDS IN FACT	OR =	37 K WORDS	NONZERO	TERMS IN FA	CTOR =	111	24 K TERMS			
SPARSE DI	COMP SUGGESTED MEMO	RY = 551	9 K WORDS								
			1	. / . (].				1	C 1)		

Use DIAG,8 to write matrix trailers (other diagnostics also useful)

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Understanding Memory in Nastran

From .f04 file:					
0 ** MASTER DIRECTORIES ARE LOADED	IN	MEMORY.			
USER OPENCORE (HICORE)	=	804908563	WORDS		
EXECUTIVE SYSTEM WORK AREA	=	316925	WORDS		
MASTER (RAM)	=	80917	WORDS		
SCRATCH (MEM) AREA	=	268443648	WORDS	(8192 BUFFERS)
BUFFER POOL AREA (GINO/EXEC)	=	268427231	WORDS	(8189 BUFFERS)

```
TOTAL NX NASTRAN MEMORY LIMIT = 1342177284 WORDS
```

Total memory is what's requested on mem= keyword (default is 45% of physical)

• Total RAM available to Nastran throughout its run time

Scratch(MEM) is what's requested on smem = keyword (default is 20% of mem)

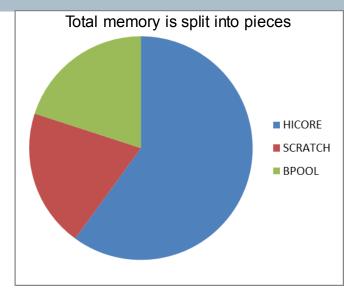
- RAM available to write scratch files before spilling to disk (very useful for slow disks/lots of RAM)
 Buffer pool is what's requested on bpool = keyword (default is 20% of mem)
- RAM available to buffer writes to scratch files (100 buffers is 50 Mbytes)

User OpenCore is what's left over for "in-core" operations (default is 60% of mem)

RAM available for memory intensive operations such as decomposition (typically not much needed)
 Maximum memory is 8 Gbytes for LP version

memorymaximum keyword sets maximum allowed memory request (default is 80% of RAM)
 Defaults work "on average" but our experience is that maximizing smem optimizes performance

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"Optimal" Memory Allocation

Typically not much advantage to allocating more memory to HICORE than required to avoid spill in decomposition step (there are some exceptions)

PARAMETERS FOR SPARSE DECOMPOSITION OF DATA BLOCK KXX (TYPE=RSP) FOLLOW	
MATRIX SIZE = 31516 ROWS NUMBER OF NONZEROES = 11864738 TEL	RMS
NUMBER OF ZERO COLUMNS = 0 NUMBER OF ZERO DIAGONAL TERMS = 0	
CPU TIME ESTIMATE = 204 SEC I/O TIME ESTIMATE = 0 SEC	
MINIMUM MEMORY REQUIREMENT = 3518 K WORDS MEMORY AVAILABLE = 1407554 K WORDS	
MEMORY REQR'D TO AVOID SPILL = <u>19946 K WORDS</u> MEMORY USED BY MMD = 3362 K WORDS	
EST. INTEGER WORDS IN FACTOR = 18846 K WORDS EST. NONZERO TERMS = 36674 K TERM	MS
ESTIMATED MAXIMUM FRONT SIZE = 3466 TERMS RANK OF UPDATE = 128	

*** TOTAL MEMORY AND DISK USAGE STATISTICS ***

+	SPARSE	SOLUTION	MODULES		+	+	MAXIMUM	DISK USAGE		+
HIWATER		1	SUB_DMAP		DMAP	HIWATER		SUB_DMAP		DMAP
(WORDS)	DAY	TIME	NAME		MODULE	(MB)	DAY_TIME	NAME		MODULE
<u>1391409310</u>	14:2	20:21	XREAD	251	READ	3850.188	14:21:11	XREAD	251	READ

For this problem maximum HICORE memory was 8*1391409310/1024^3=10.4 Gbytes (that's a lot)

- This particular problem includes fluid mass that results in a very dense mass matrix
- Most solutions in Nastran actually don't require that much (only 155 Mbytes required to avoid spill in above example)
 To calculate memory start from total and leave maximum amount for smem:
- 80% of physical is 25.6 Gbytes (mem = 25.6 gb) same as memorymaximum default
- Buffpool of 100 blocks is 50 Mbytes not much advantage beyond that
- 10.5 Gbytes required for HICORE, so about smem=15 gb is optimal





Look at Bottom of .f04 for Database Usage

*** DATABASE USAGE STATISTICS ***

+	LO	GICAL DBSETS		+	+		DBSET FI	LES	+
DBSET	ALLOCATED	BLOCKSIZE	USED	USED	FILE	ALLOCATED	HIWATER	HIWATER	I/O TRANSFERRED
	(BLOCKS)	(WORDS)	(BLOCKS)	Ŷ		(BLOCKS)	(BLOCKS)	(MB)	(GB)
MASTER	5000	65536	42	0.84	MASTER	5000	42	10.500	0.290
DBALL	2000000	65536	3	0.00	DBALL	2000000	3	0.750	0.004
OBJSCR	5000	8192	285	5.70	OBJSCR	5000	285	8.906	0.016
SCRATCH	4000100	65536	19	0.00	(MEMFILE	100	100	25.000	0.000)
					SCRATCH	2000000	450748	112687.000	1017.365
					SCR300	2000000	4883	1220.750	11.971
								TOTAL	: 1029.645

- Size in GBytes = BUFFSIZE*BLOCKS*BYTES/WORD/1024³
 - Maximum BUFFSIZE is 65537 (recommended for large runs)
 - Recommendation is maximum for more than 400,000 DOF
 - Bytes/Word is 8 for ILP and 4 for LP
 - Above example has limit of 2,000,000*65,537*8/1,024³=976.6 GBytes allocated to DBALL
 - Allocation is logical limit, not related to actual disk space available
 - Maximum size of SCRATCH+SCR300=222.5 GBytes
 - Total I/O to SCRATCH+SCR300>1 Terabyte (in 14 minutes on a desktop)



Summary of Terms so Far

- LP long precision version of Nastran (32 bit integers)
- ILP Integer long precision version of Nastran (64 bit integers)
- WORD 4 bytes for LP version and 8 bytes for ILP version
- BUFFSIZE Number of words in a block
- BLOCK (Buffsize words 65536*8 = 512 Kbytes)
- SMEM Memory reserved to "write" scratch files
- BPOOL Memory reserved to cache writing of scratch files
- **HICORE** Memory reserved for in-core operations
- SCRATCH File used by Nastran to store intermediate data
- SCR300 Scratch file used for temporary storage within a module
- DBALL Database file used to store data for restart
- DMAP Language that Nastran solution sequences are written in

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How Do You Control I/O?

- Files can be controlled with INIT cards in input deck
- Easier to control by keywords on nastran submittal or RCF file
 - System .rcf file in Nastran installation (e.g. .../conf/nast9rc or ...\conf\nast9.rcf)
 - Hierarchy of .rcf files (system, architecture, node, user, local)

Keyword	Interpretation		
Buffsize	BUFFSIZE in blocks		I/O Speed
dbs	Location of MASTER/DBALL files	Typical .rcf file	<u>I/O Speeu</u>
sdball	Logical size limit of DBALL file	Buffsize=65537	RAM 🔶 Faster
sdir	Location of SCRATCH/SCR300 files	dbs=S:\scratch sdball=500gb	Local SSD
sscr	Logical size limit for SCRATCH/SCR300	sdir=S:\Scratch	Local HD
scr	What gets written to DBALL file (yes, no, mini)	sscr=200gb	Network Slower
smem	RAM allocated to SCRATCH/SCR300	scr=no	
mem	Total RAM allocated to run		
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- Largest amount of I/O is to SCRATCH and SCR300 file
 - If you have LOTS of RAM (100+ GBytes) use smem to allocate some portion of total memory (mem) to SCRATCH
 - mem=200gb, smem=190gb allocates 190 GBytes to SCRATCH, 10 to solver
 - If you don't have enough RAM to fit entire SCRATCH/SCR300 files make sure that these are written to a fast local disk
 - Solid state disks are faster than spinning disks (SSD's not created equal)
- If you want general RESTART use scr=no to save max data to DBALL
 - Make sure that DBALL is on fast disk
- If you want just data recovery RESTART use scr=mini
 - Location of DBALL less critical
- If you don't want to RESTART use INIT MASTER(S) (default in FEMAP)





Anatomy of Nastran Direct Static Solution

- 1. Generate elemental matrices KELM, KDICT (EMG)
- 2. Assemble elemental matrices KGG (EMA)
- 3. Reduce down to L-set KLL (MCE1/MCE2, etc.)
- 4. Solve equations KLL*UL=PL (DCMP and FBS)
- 5. Expand results to G-set UG (SDR1)
- 6. Calculate outputs OUGV, OES etc. (SDR2)

For most problems the solve step is the most expensive (only step that Nastran runs in parallel using SMP)

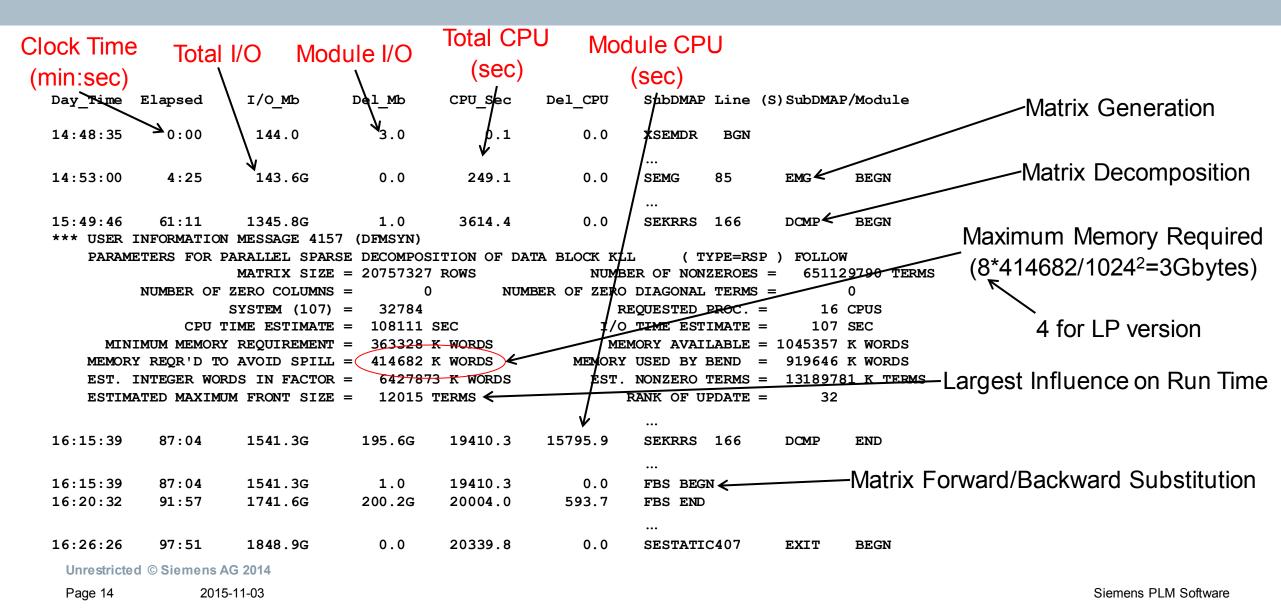
The reduction and expansion steps (3 and 5) are largely matrix multiplies. (For some solutions these can become expensive)

Output processing (step 6) can get expensive if LOTs of outputs are requested (e.g. GPFOR or STRESS on entire model)





Anatomy of .f04 File for a Direct Static Solution







What Can be Done to Speed up Direct?

Solution time is most sensitive to FRONT SIZE

Defaults work OK for most/many problems

Try modifying DCMP reordering algorithm (default is BEND (EXTREME), but METIS is sometimes better)

• NASTRAN DCMPSEQ=8 (or 9)

Check to see if FRONTSIZE decreased

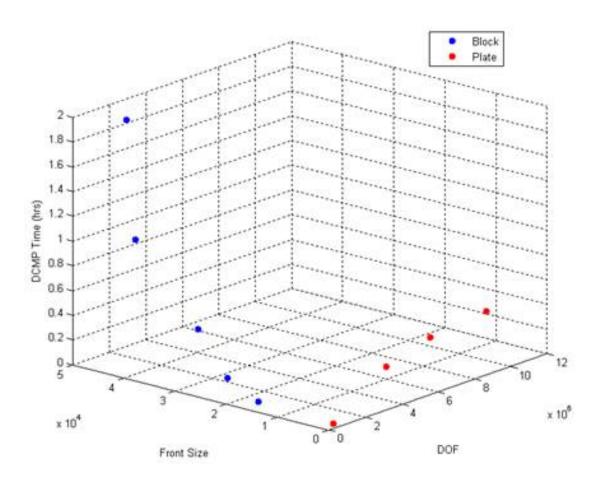
Use scr=mini to store LLL on scratch rather than DBALL (also results in much smaller DBALL and is the default we use in our .RCF file for the HPC machine)

This only helps speed is SCRATCH file has faster I/O than DBALL
 Use larger value of BUFFSIZE (Can set this in the .rcf file by default)
 Give Nastran the most amount scratch memory (smem) you can

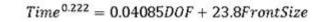
- smem comes out of mem so to get 190 GBytes of smem and 16 GBytes of memory you need mem=206GB, smem=190GB (new SNAS script does this)
- In our experience Nastran is able to get about 80% of available RAM on Linux
- If you don't have enough RAM it will spill to disk. This can be slow if scratch disk is slow.



Solution Time Much More Sensitive to Front Size Than # DOF



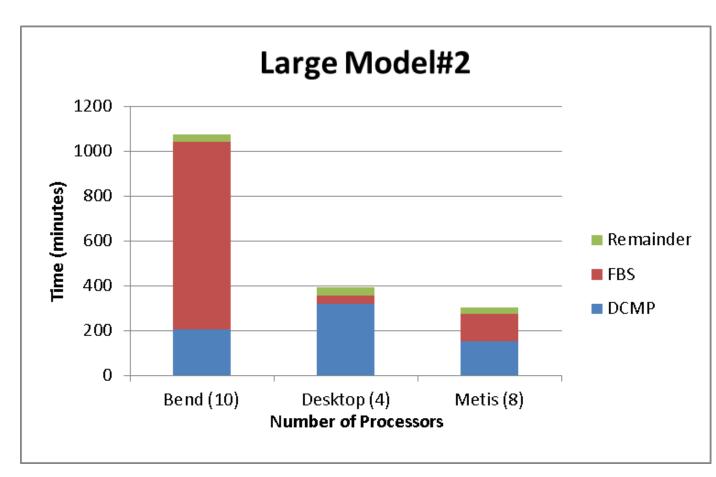
- "Blocky" models tend to have larger Front Size for given # of DOF
- Run time is fairly low with > 10 million DOF as long as Front Size remains low
- Run time increases very rapidly with increasing Front Size even with relatively low number of DOF





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Example Where Switching Reordering Helped



Forward-Backward Substitution was really slow with default Bend ordering.

Default BEND ordering – FS = 57,669

METIS ordering -FS = 51,948 (10% less)

(DCMPSEQ=8, or 9)

Run time decreased by > 3x with fewer processors

Performance is VERY job specific

Changing reordering is something to try





Iterative Solver Can Sometimes be MUCH Faster

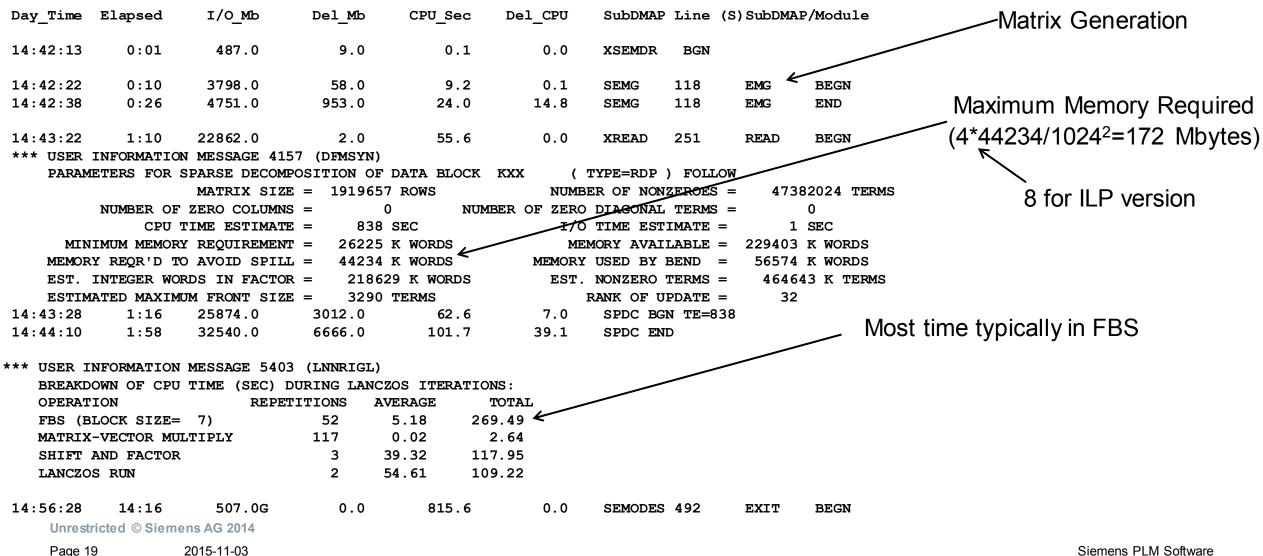
- Iterative solution is usually fastest way of speeding up static solution (for small number of load cases)
- Skips matrix assembly, decomposition and forward/backward substition
- Longest step is typically matrix generation (EMG)
- e.g. large solid model (front size=53,532) with 1 load case reduced from 226 to 20 minutes
- NASTRAN ITER=YES, ELEMITER=YES
- ITER, 100, ITSEPS=1E-10 (improves accuracy at very little extra cost)

Clock Time	Tota	I I/O	Module I/O	Total CPU (sec)	J Moc	lule CP	U			
(min:sec)		\mathbf{N}		· · · · ·		(sec)				
Day_Time	Elapsed	\ 1/0_M	o Dell_Mb	CPU_Sec	Del_CPU	Subdmap	Line	(S) SubDMAP	/Module	Matrix Generation
	\sim	\mathbf{N}	×	1						
20:44:39	A0:06	880.0) 19.0	. (1 . 0	0.0	XSEMDR	BGN			
		N N		V		/				
20:46:35	2:02	51238.0	0 1.0	114.9	0.0 /	SOL2	178	EMG 🛩	BEGN	
21:01:49	17:16	62745.0	0 11507.0	1026.0	911.2/	SOL2	178	EMG	END	
21:02:06	17:33	75156.0	0 1.0	1041.0	010	SOL2	354	SOLVIT	BEGN	
21:04:55	20:22	87615.0) 12459.0	1570.5	529.5	SOL2	354	SOLVIT	end 🔶	Iterative Solution
21:05:10	20:37	91510.0	0.0	1585.0	0.0	SOL2	591	EXIT	BEGN	(< 9 minutes!)



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Modal Solution Typically Dominated by READ Step



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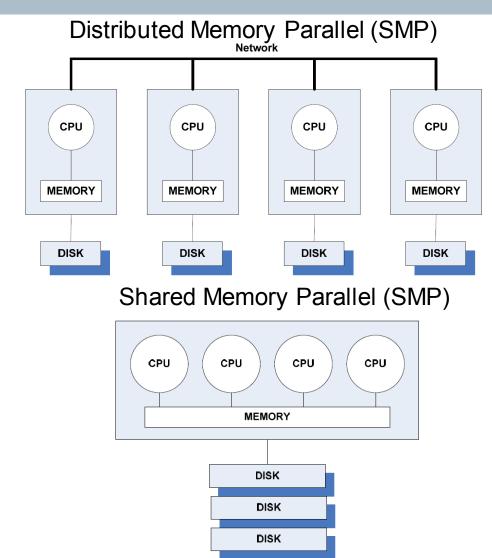
What Have We Learned So Far?

- For Nastran I/O is king
- I/O to SCRATCH and SCR300 files is typically most important
 - Amount of I/O to DBALL file controlled by scr keyword (yes, no, mini)
- RAM is fastest I/O \rightarrow Using smem to allocate RAM to scratch can be VERY effective
 - Only works with LARGE amounts of RAM (256 GBytes/node on our HPC cluster)
- If you don't have enough RAM, fast (i.e. SSD) local disk is critical
- You typically need much less RAM to solve than you might think
 - Throwing lots of RAM without using smem is typically <u>not</u> effective
 - Look at "minimum to avoid spill" and round up to get reasonable RAM
 - Remaining RAM is best left to OS or used for smem
- If direct static solution seems long try METIS ordering (DCMPSEQ=8 or 9)
- Try using iterative solver for statics with small number of load cases
- Use .f04 file to understand where job is using time
 - EMG, (DCMP for statics and READ for modes) good points to look at solution
- No one set of options appears to be optimal for all problems
 - Defaults are good for most problems



SMP vs DMP in NX Nastran

- SMP works on any computer with multiple processors
 - Including almost all desktops
 - A single node of an HPC cluster
 - smp = n, or parallel = n
 - Fine grain parallelism only applies to specific steps
 DCMP, FBS, SOLVIT
 - Easy, but of limited benefit
 - Limited benefit above n=4 in our experience
- DMP works on a network of computers
 - Typically multiple nodes on HPC cluster
 - dmp = n (nrec = n, dstat = n, numseg = n, nclust = n)
 - Coarse grain parallelism divides problem into multiple subproblems
- SMP and DMP can be combined
 - Subdivide at a coarse level, and have each sub-problem solve faster with SMP

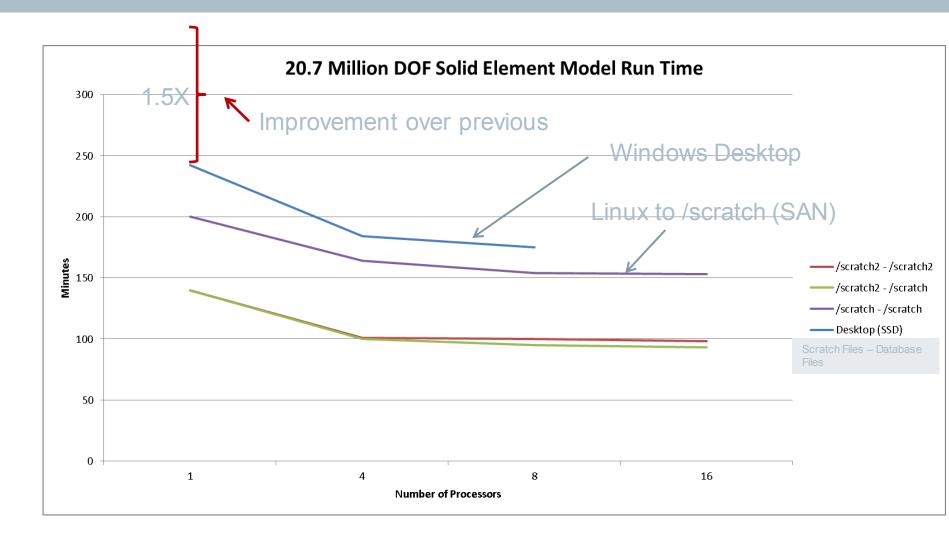


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Example of SMP Performance

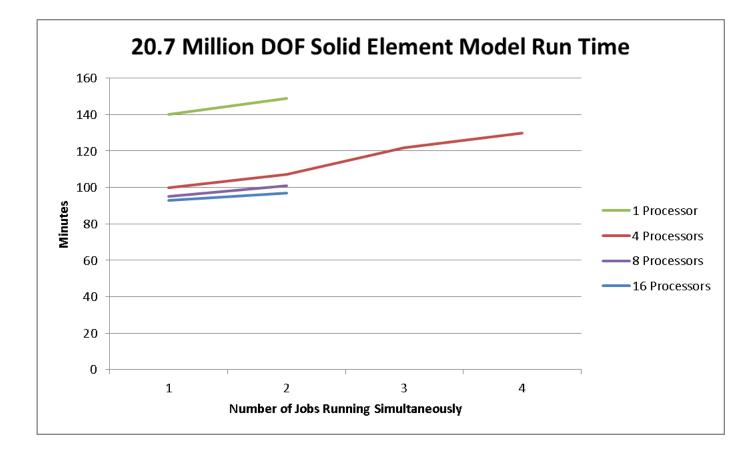


- Performance is VERY problem specific
- Speedup is rarely anywhere close to linear
- Throughput usually better with multiple jobs
 - Within limits
- Performance more sensitive to disk than smp
- Don't be fooled by looking at CPU usage during run





Multiple Runs on Single Node Provides Better Throughput



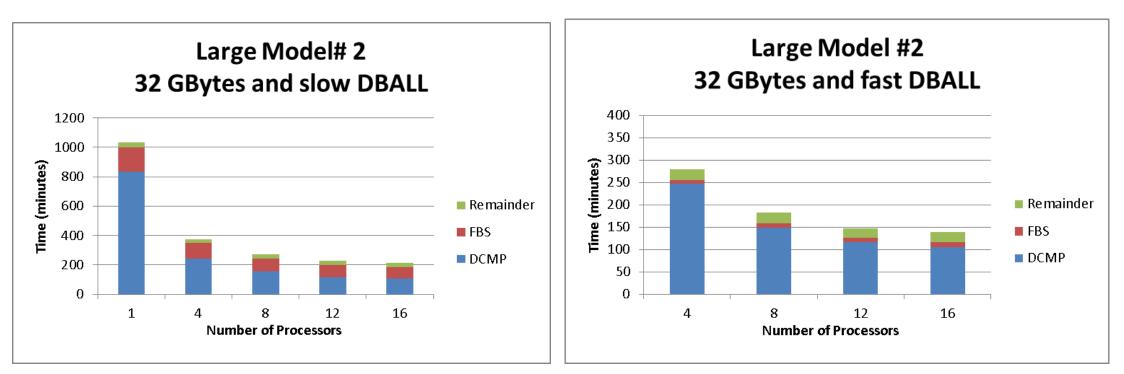
Performance very job specific (single job run time optimal with 1 job)

- ~10% penalty for 2 jobs
- ~20% penalty for 3 jobs
- ~30% penalty for 4 jobs (total throughput optimal with 4 jobs)
 - Assumes number of licenses not an issue





Different Model Scales Better with Processors



New Conclusion: for this Class of Model (Higher Front Size) When the Front Size is High, the ordering and the DBALL speed and the number of processors matters!



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Lots of Different DMP Methods in NX Nastran

Solution	Method	Command	Suggested Model Type
101	GDSTAT	dmp=p	Large models
		dmp=p,	Smaller models, large
101	LDSTAT	dstat=1	number of laods
		dmp=p,	Small models, large
103	FDMODES	numseg=p	number of frequencies
			Large models, small
103	GDMODES	dmp=p	number of frequencies
		dmp=p,	Large models, large
103	HDMODES	nclust=c	number of frequencies
		smp=p,	Large models,
103	RDMODES	nrec=n	approximate solution
108	FDFREQR	dmp=p	All models

Solution Sequence SOL SOL SOL SOL 103 101 108 111 112 200 **FDMODES FDMODES FDFREQR** GDSTAT Computational Method (DMP) **GDMODES GDMODES** LDSTAT **HDMODES HDMODES RDMODES RDMODES**

FINITE ELEMENT MODEL

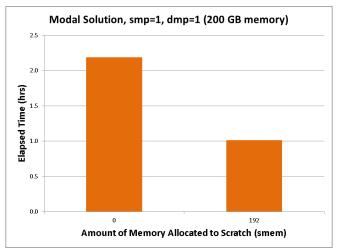
- Pre-requisites for DMP
 - NXN on all hosts
 - MPI (mpirun) available
 - Input data file visible to all hosts
 - rsh, rcp, rlogin must work to communicate among nodes
 - scp and ssh must work to remotely log into nodes Unrestricted © Siemens AG 2014

FDFREQR

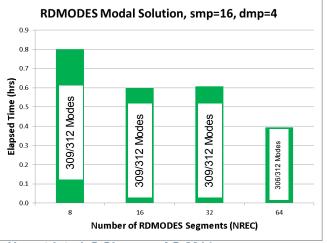


Results for RDMODES/DMP Solution (NXN 10 pre-release)

Allocating RAM to smem Halves Run Time



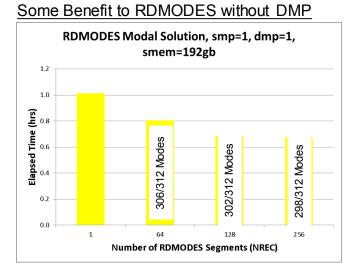




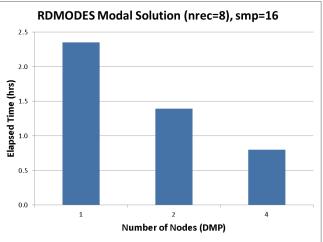
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RDMODES is an approximate method for calculating modes

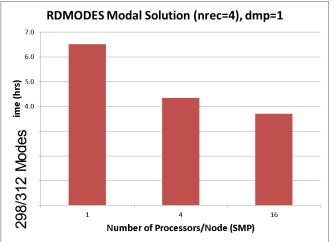
- Breaks model into successively smaller pieces (AMLS)
 - Number of pieces controlled by nrec keyword (128 256)
- rdscale keyword increases accuracy with computational cost
- Works particularly well with DMP (doesn't need to be DMP)
- Can be used for modal transient (109) or FRF (112)



Using more DMP nodes is more beneficial



Using more SMP processors has marginal benefit



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Summary

- Biggest performance gain in NX Nastran is through fast I/O
 - RAM (smem) fastest followed by local SSD
- Learn to read the .f04 file to understand performance
- Lots of solution options can be used to improve performance
 - Consider iterative solution for statics with small number of load cases
 - Consider RDMODES for modes independent of SMP/DMP
- SMP is fine grain parallelization on a single node
 - Applies equally well to a desktop
 - Very easy to use
 - Provides some advantage but doesn't scale well
- DMP is coarse grain parallelization across multiple nodes on a cluster
 - Only applicable on a cluster
 - Much more difficult to use (many different options)
 - Can scale much better than SMP