Best practices for efficient HPC performance with large models

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CADFEM

University of Ljubljana
Faculty of Mechanical Engineering

CAPACITIES

e-infrastructure

Agenda

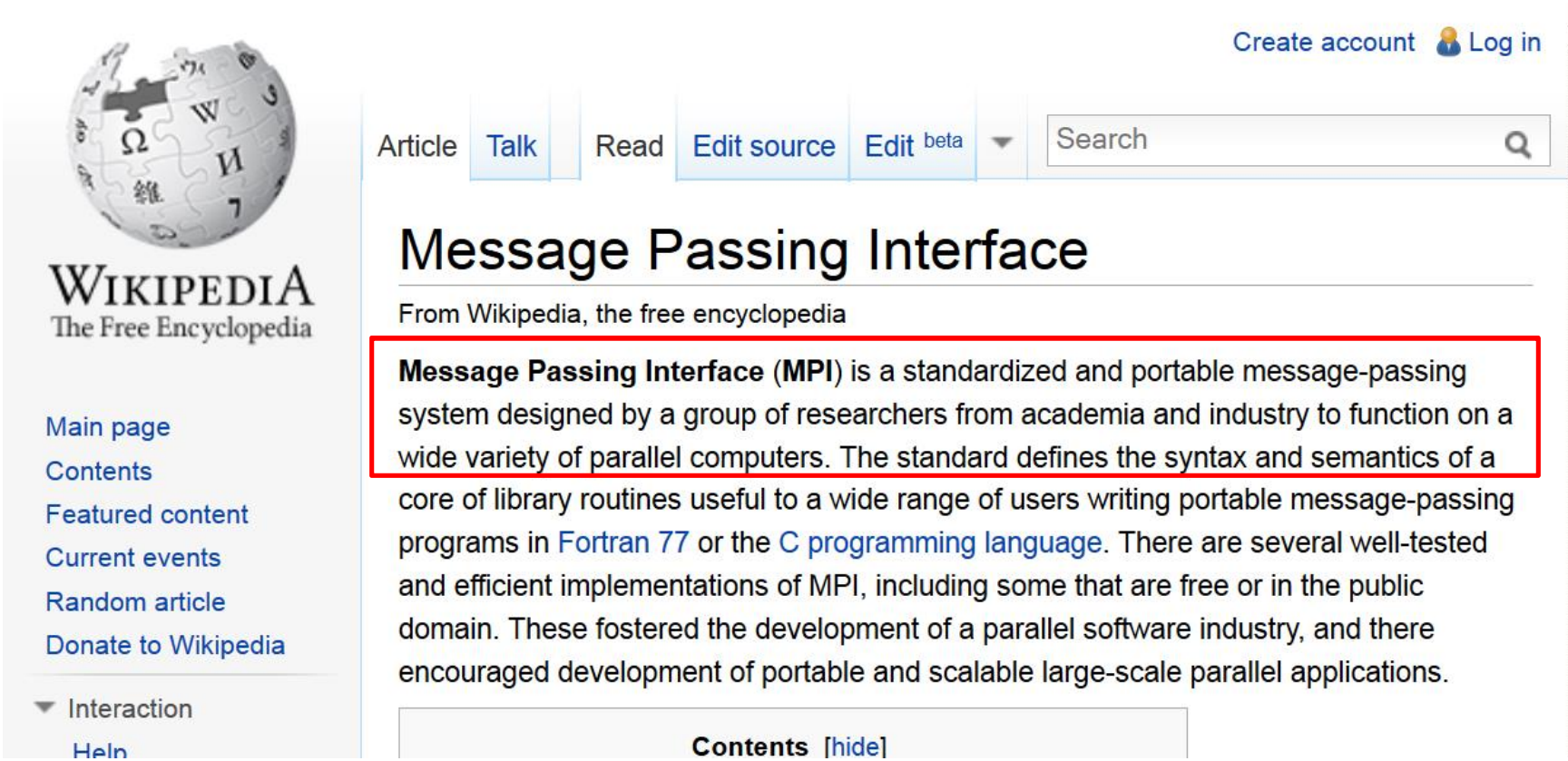
- Part I:
  - Prerequisites
    - MPI – HP or Intel
    - Hyperthreading and ANSYS
  - How to Set up HPC
    - The Remote Solve Manager (RSM)
    - Solver Handler, Number of CPUs, SMP, and DMP
    - ANSYS Mechanical APDL
  - Handling of Large Models
    - CAD Import
    - Named Selections
    - Tree Filter and Tags
    - Object Generator

Agenda

- Part II:
  - Mesh Controls for Large Models
    - Curvature and Proximity
  - How to Cut Analysis Time
    - Contact Settings
    - Analysis Settings
  - Evaluation of Results
    - Results Tracker
    - Newton Raphson Residuals and RSM
    - Postprocessing Command Snippets
    - Max Tag Adjust to Visible

Part I

Prerequisites: MPI ï HP or Intel



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Message Passing Interface

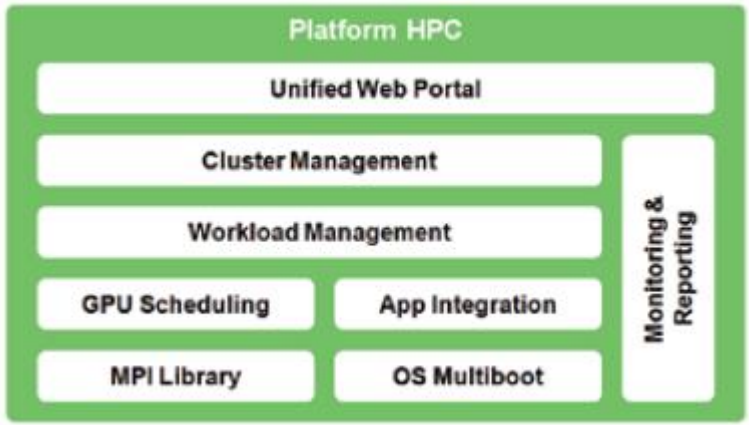
From Wikipedia, the free encyclopedia

Message Passing Interface (**MPI**) is a standardized and portable message-passing system designed by a group of researchers from academia and industry to function on a wide variety of parallel computers. The standard defines the syntax and semantics of a core of library routines useful to a wide range of users writing portable message-passing programs in Fortran 77 or the C programming language. There are several well-tested and efficient implementations of MPI, including some that are free or in the public domain. These fostered the development of a parallel software industry, and there encouraged development of portable and scalable large-scale parallel applications.

Contents [hide]

Prerequisites: MPI ï HP or Intel

- IBM Platform (HP) MPI is a little more robust than Intel MPI.
- if both can solve, it seems Intel MPI is a little faster (1% or 2%) than Platform MPI.



Source: IBM

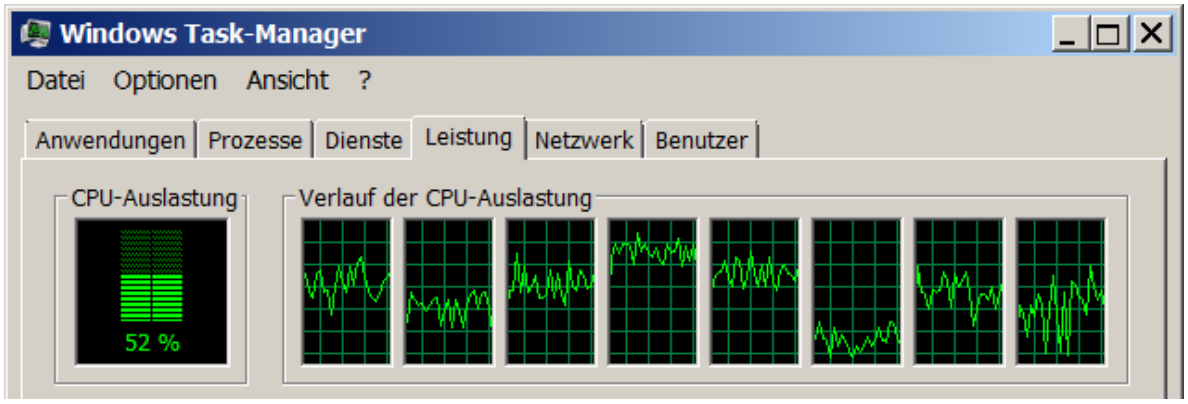
Prerequisites: Hyperthreading and ANSYS

- Ansys **doesn't do** any distinction between physical processors (e.g. 2x Xeon processors on two separate sockets) and virtual processors (i.e. cores), and between virtual processors (cores) and logical processors (if you have Hyperthreading enabled, this would "double" the cores you have).
- This might cause some troubles -> next slide

Prerequisites: Hyperthreading and ANSYS

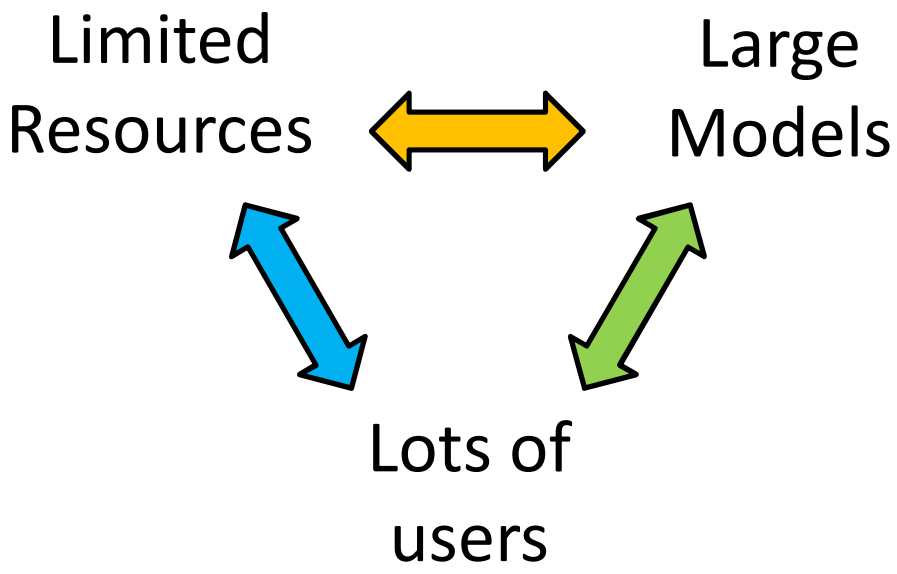
- E.g. running a job on 8 cores with activated hyperthreading would results in the following warning during the solution:

*** WARNING *** CP = 0.499 TIME= 17:04:40
The requested number of shared-memory processors (8) exceeds the number of physical processors that are available (4). As the use of virtual processors is not recommended, the number of processors used will be 4.



How to Set up HPC ï The RSM

Å Why RSM?



How to Set up HPC ï The RSM

- ***Client:*** Computer, used for Pre- and Postprocessing
- ***Job:*** Simulation
- ***Compute Server:*** these are the machines on which jobs are run
- ***RSM* (Remote Solve Manager, aka: RSM Host):** dispatches jobs to computing resources
- ***Queue:*** A queue is a list of Compute Servers available to run jobs

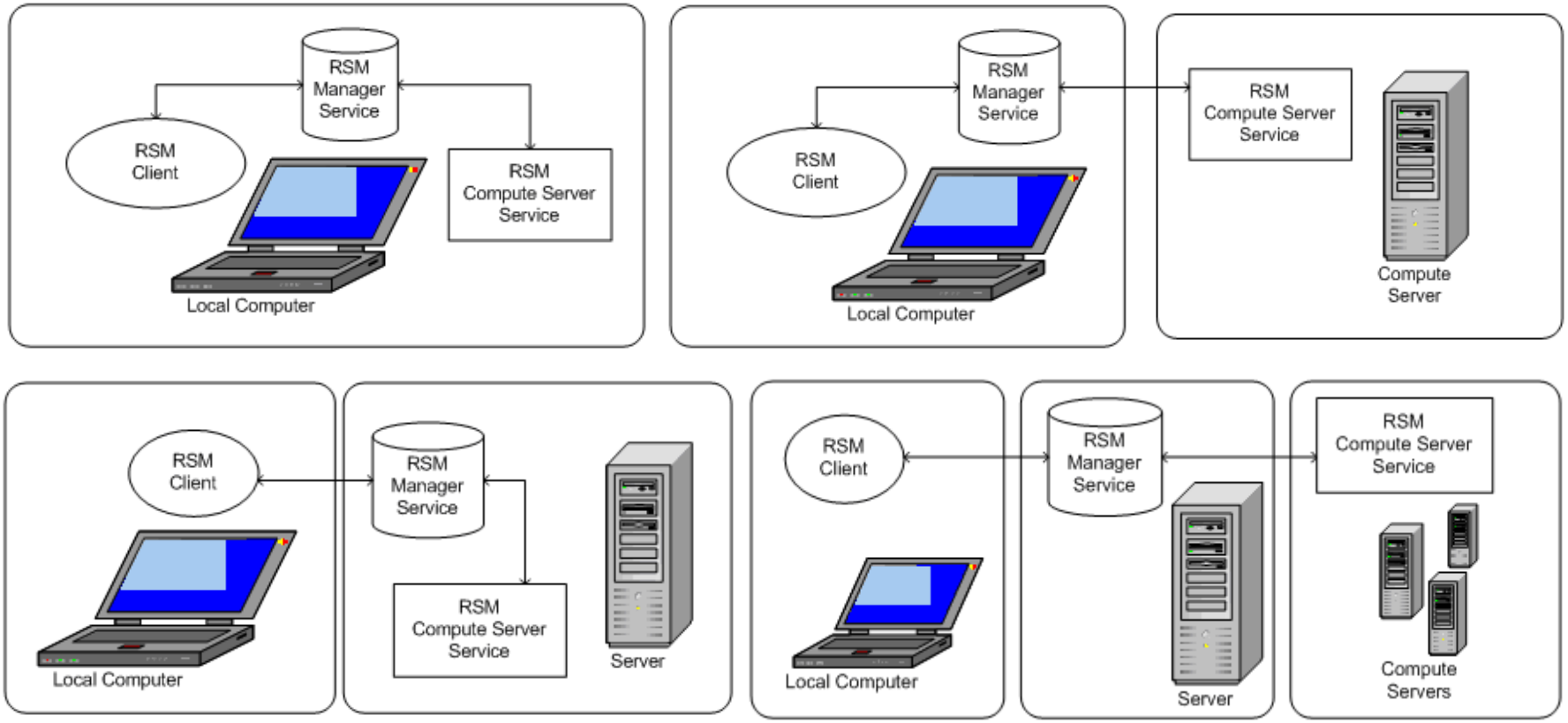
How to Set up HPC ï The RSM

Å ***Efficient use of licenses***

- ï ***Single license:*** one license can be used for all tasks at a time
- ï ***Split license:*** split of the license in Pre-Post and Solve-Batch. During solution the Pre-Post license can be used to prepare the next simulation or for postprocessing.

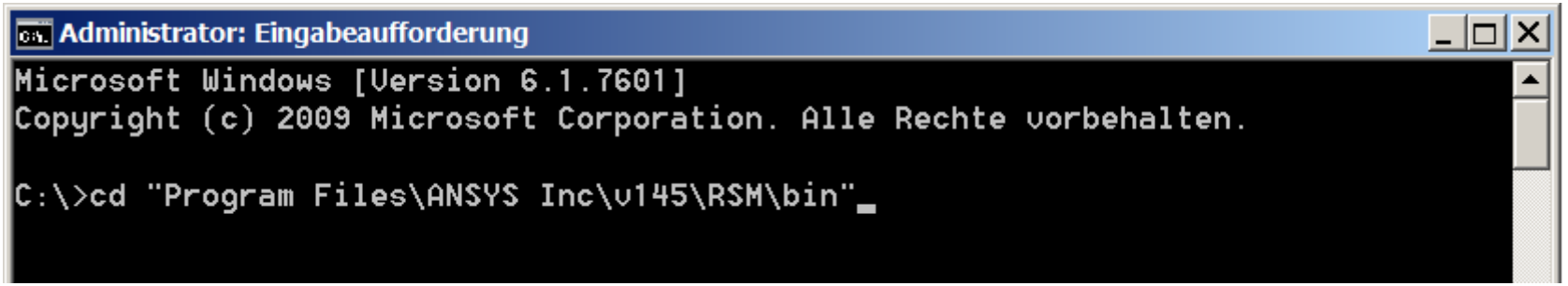
How to Set up HPC ï The RSM

Å Different system configurations

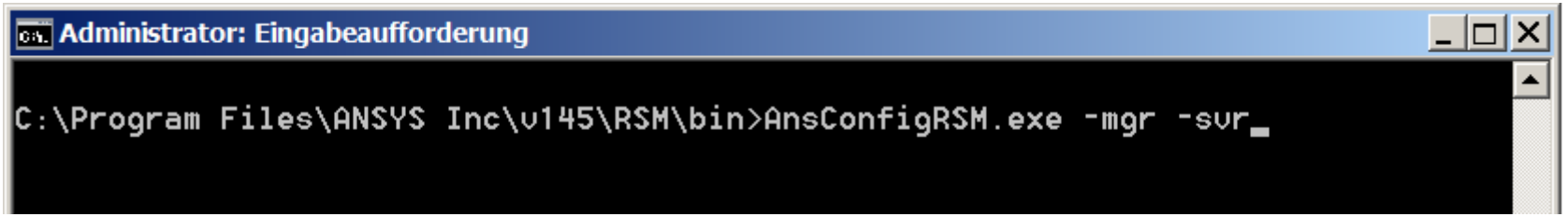


How to Set up HPC ï The RSM

- Login as **Administrator** and change Dir to install folder ANSYS



- Install Manager and/or Server service



How to Set up HPC ï The RSM

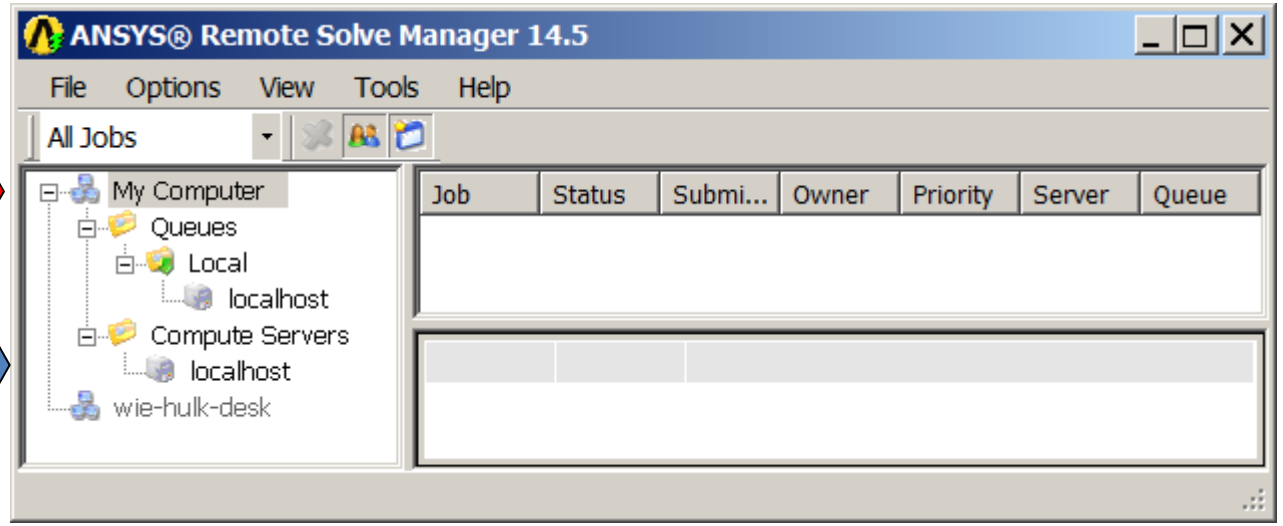
Å Start RSM:

ANSYS 14.5: Start > Programme > ANSYS 145 > Remote Solve Manager

RSM Manager

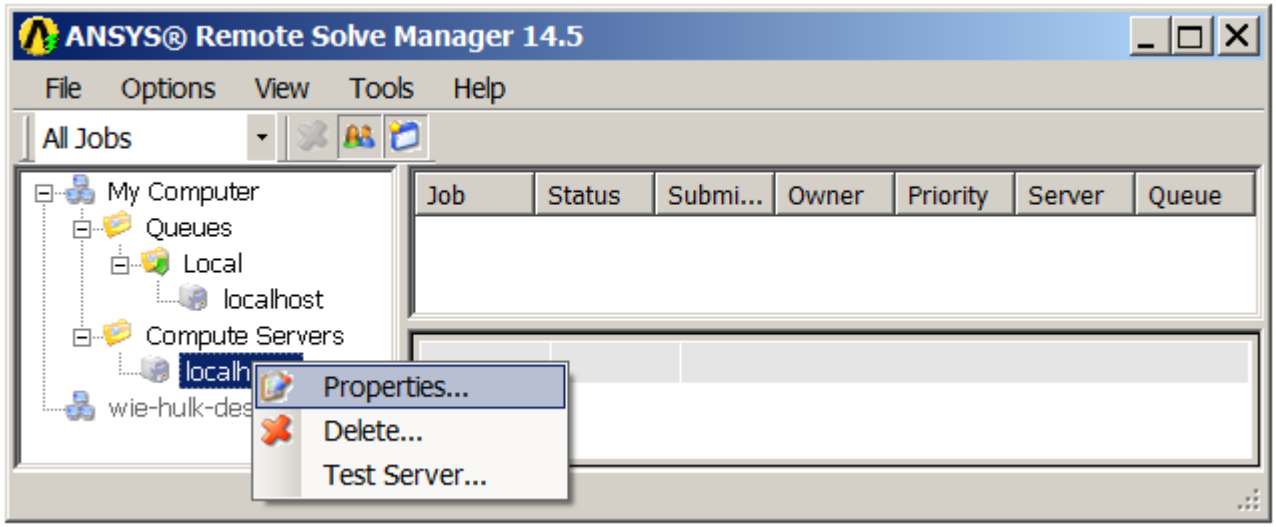
Queues

Compute Server



How to Set up HPC ï The RSM

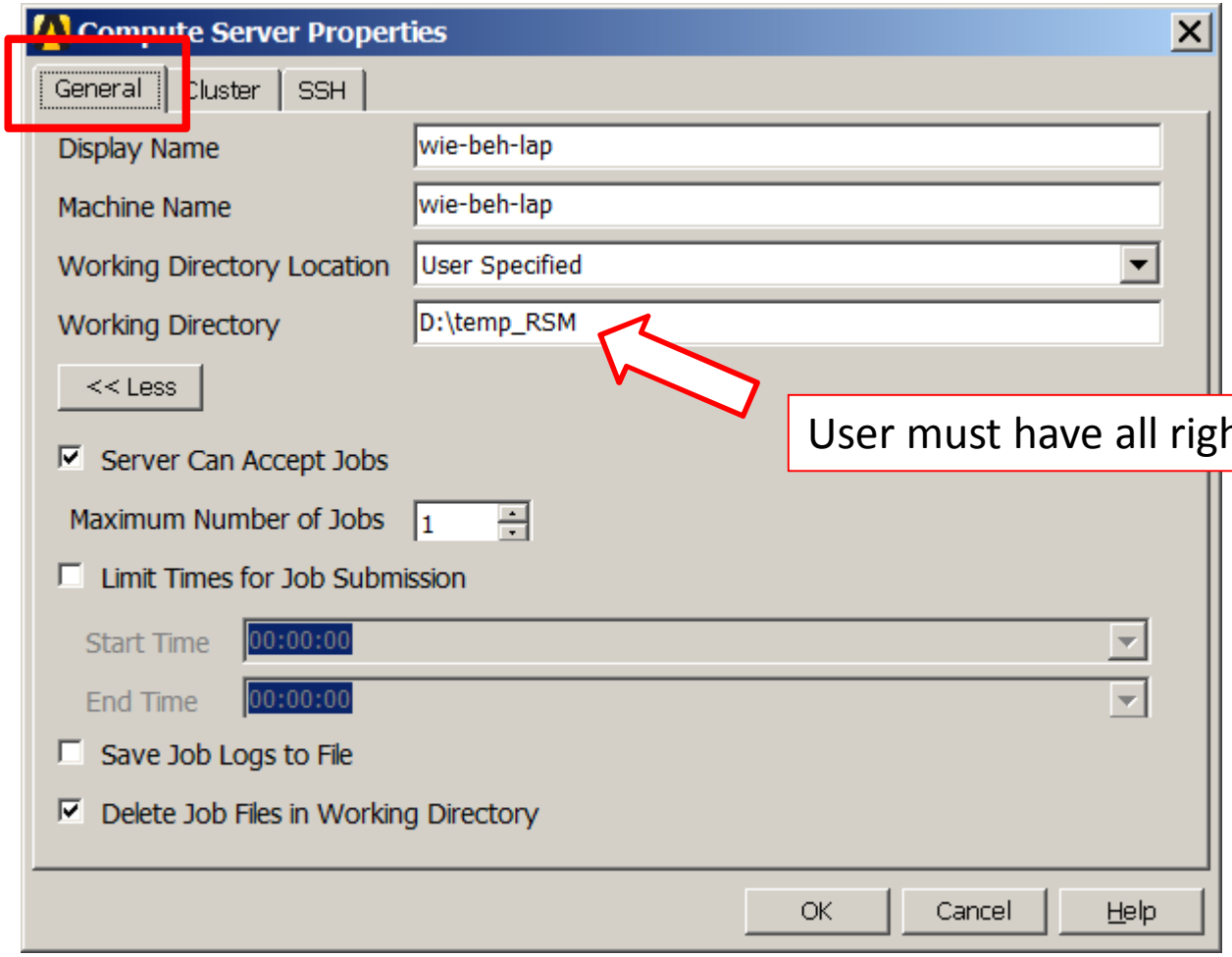
Å Setup RSM:



RMB

How to Set up HPC ï The RSM

Å Setup RSM:



How to Set up HPC ï The RSM

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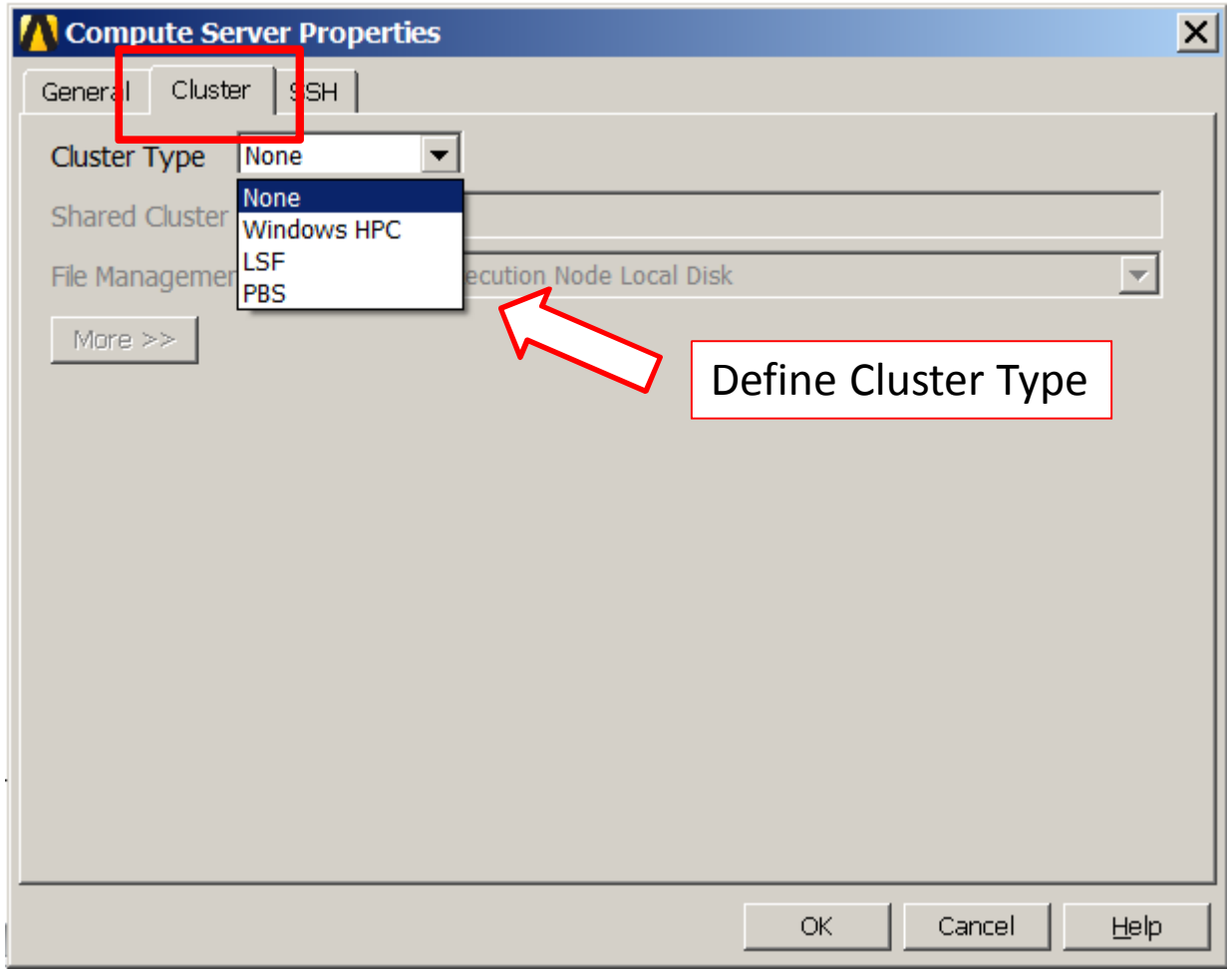
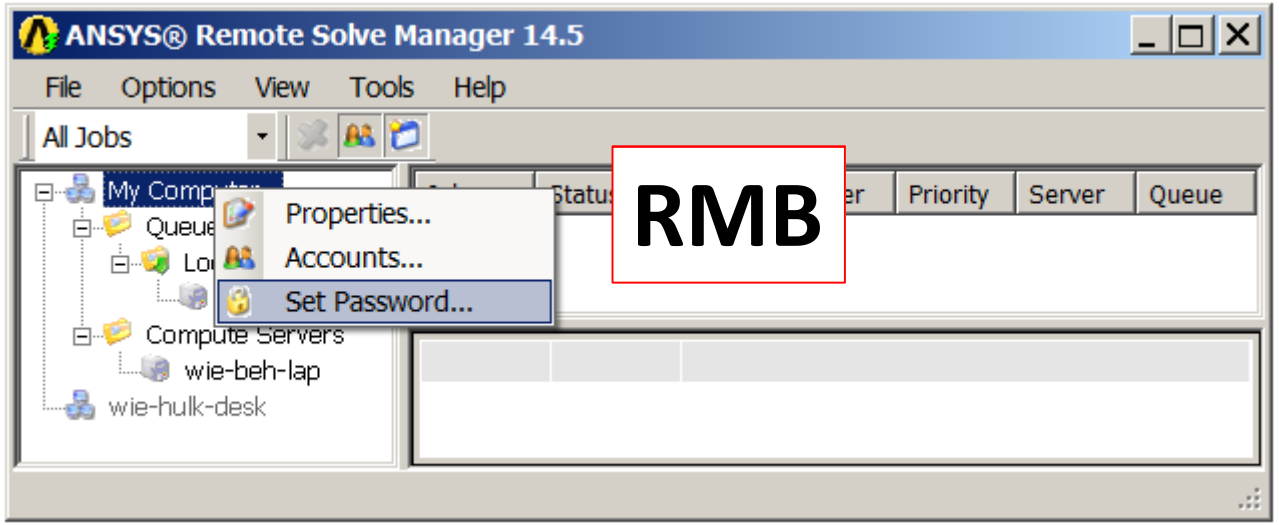


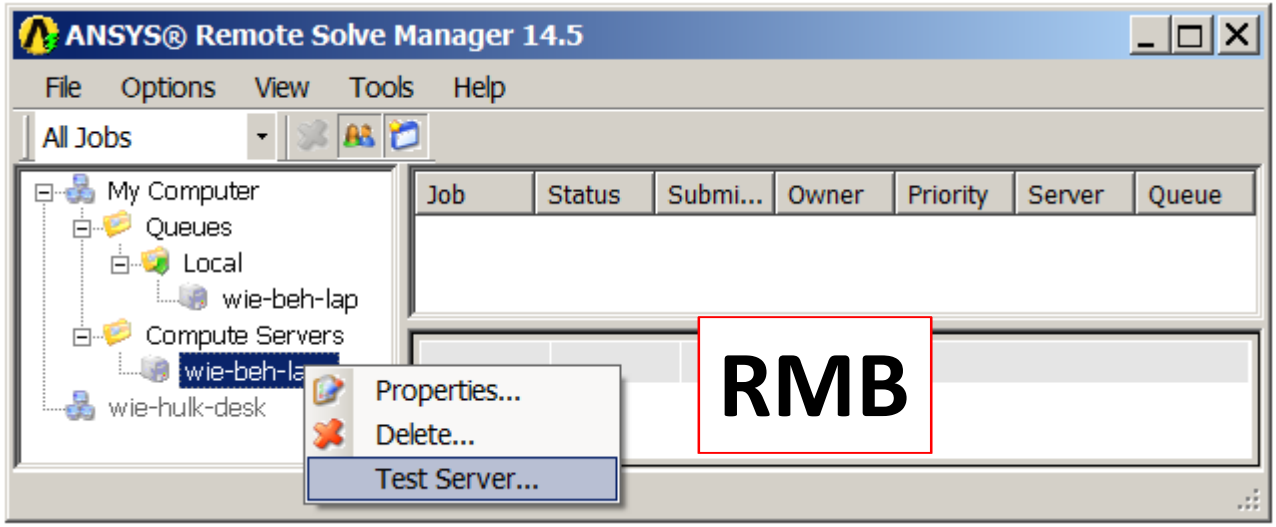
How to Set up HPC ï The RSM

Å Set your Password (your login)



How to Set up HPC ï The RSM

Å Test the Server



How to Set up HPC ï The RSM

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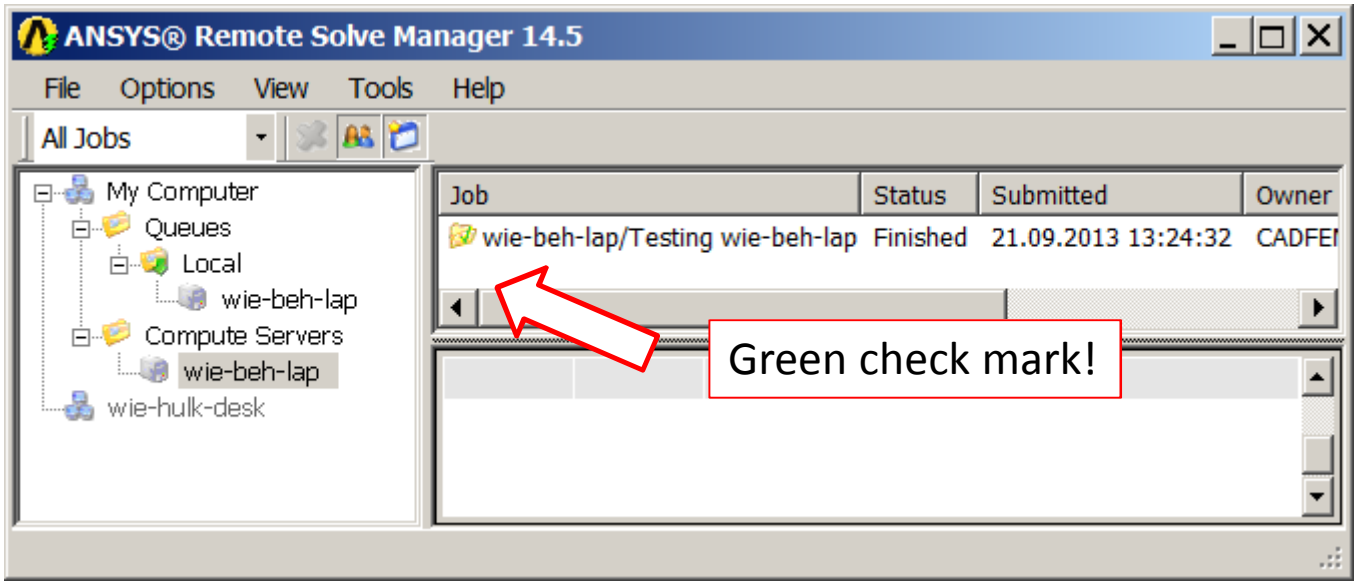
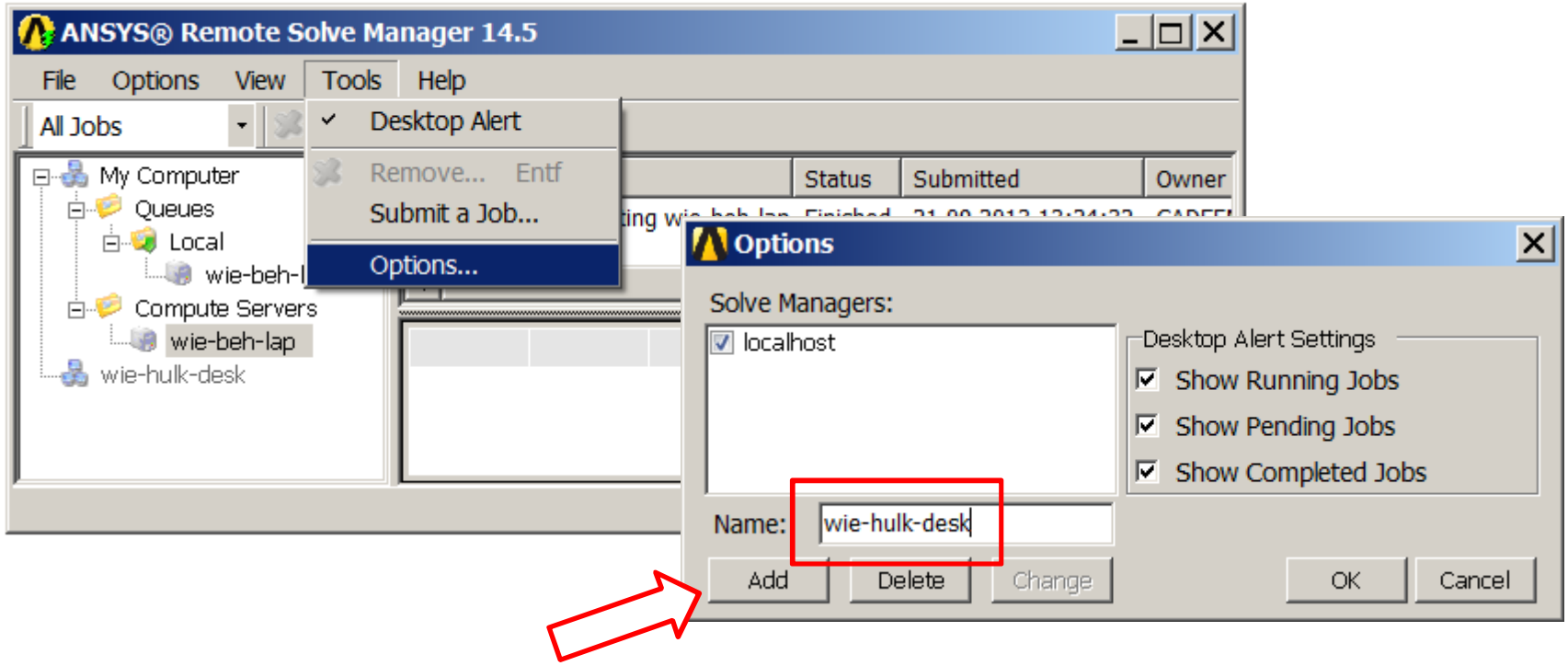


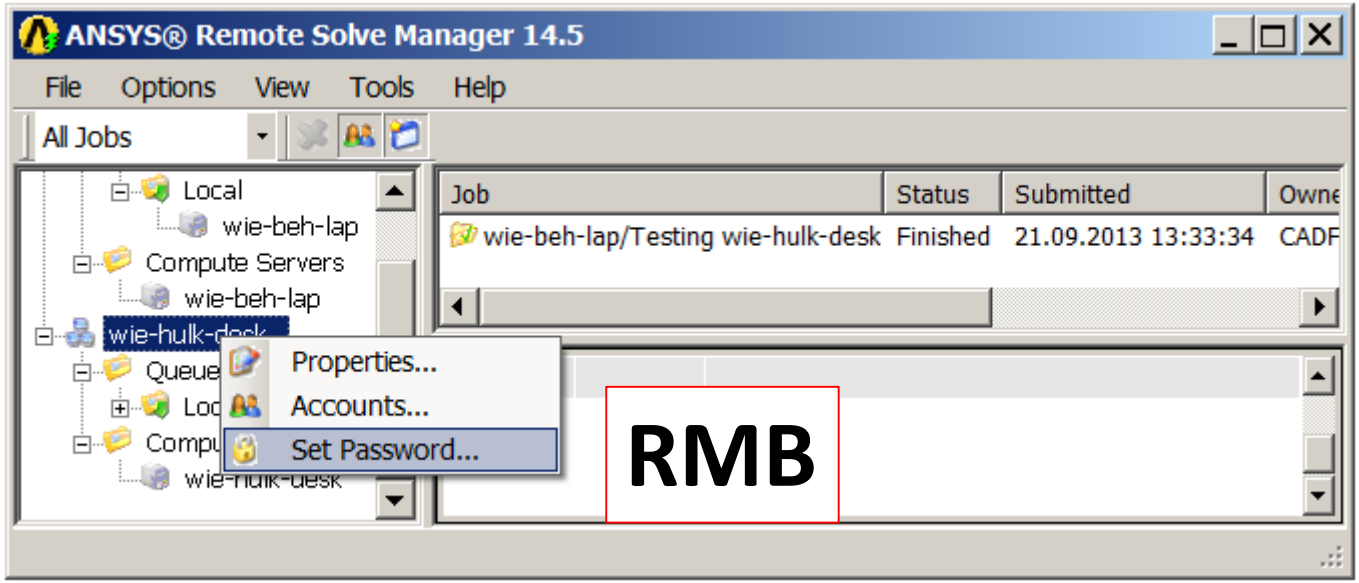
How to Set up HPC ï The RSM

Å Add a RSM manager



How to Set up HPC ï The RSM

- Add a RSM manager
  - Set your Password (your login)



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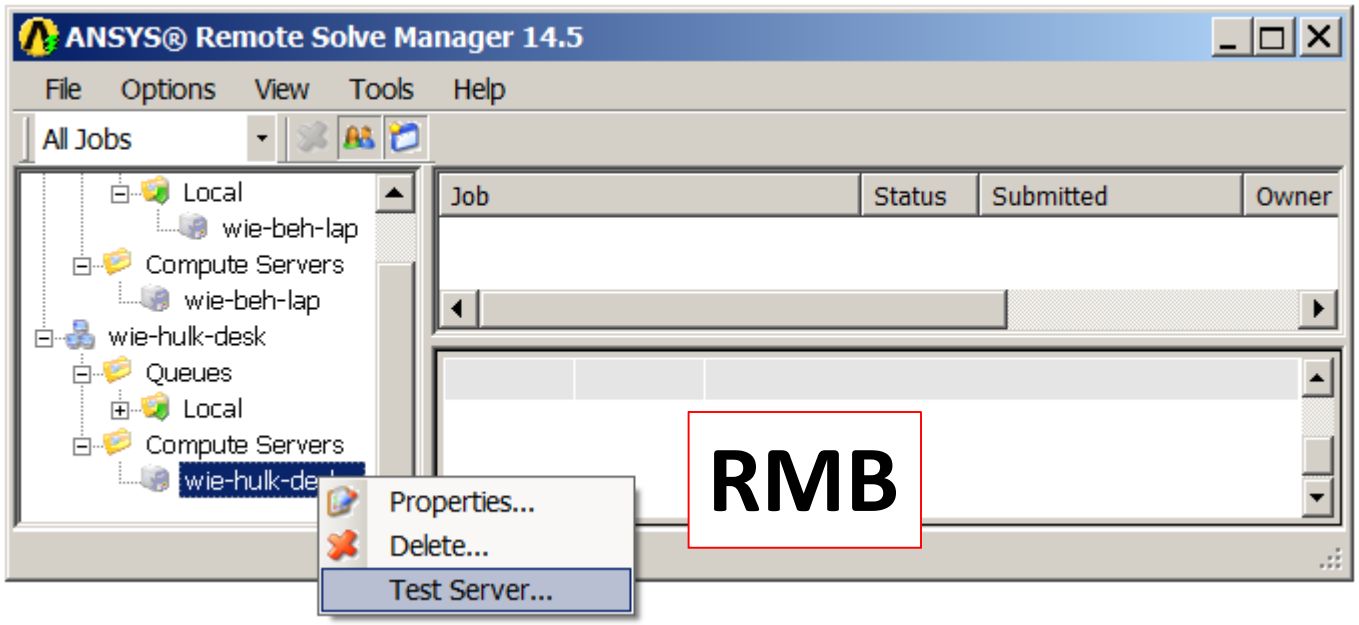

How to Set up HPC ï The RSM

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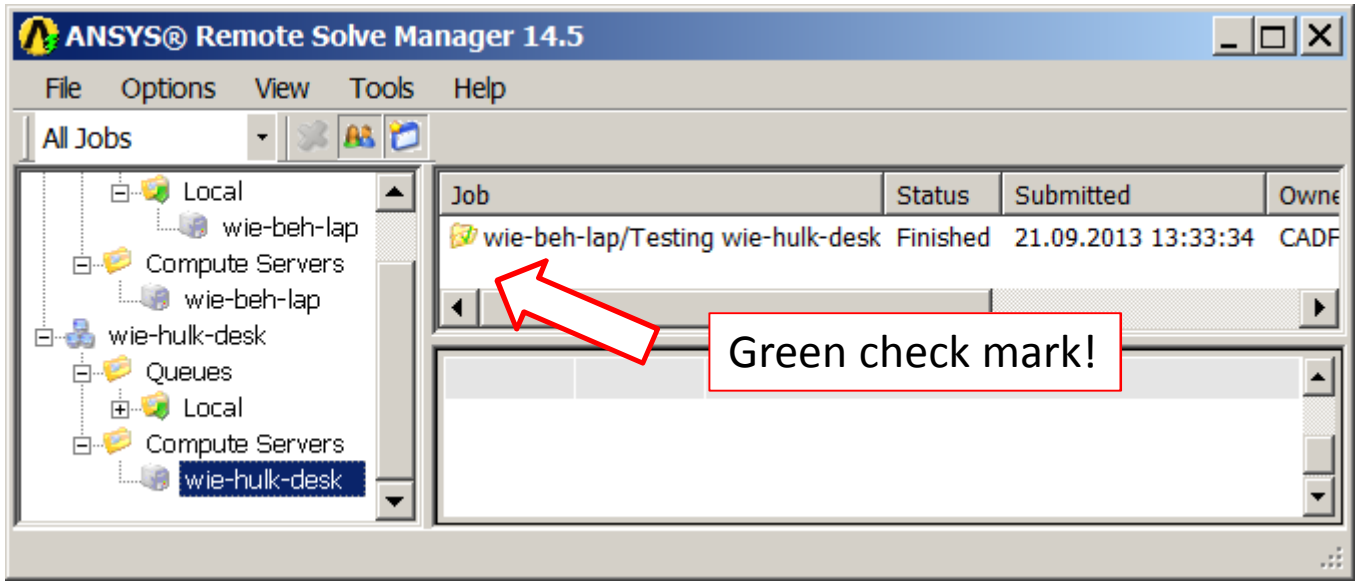


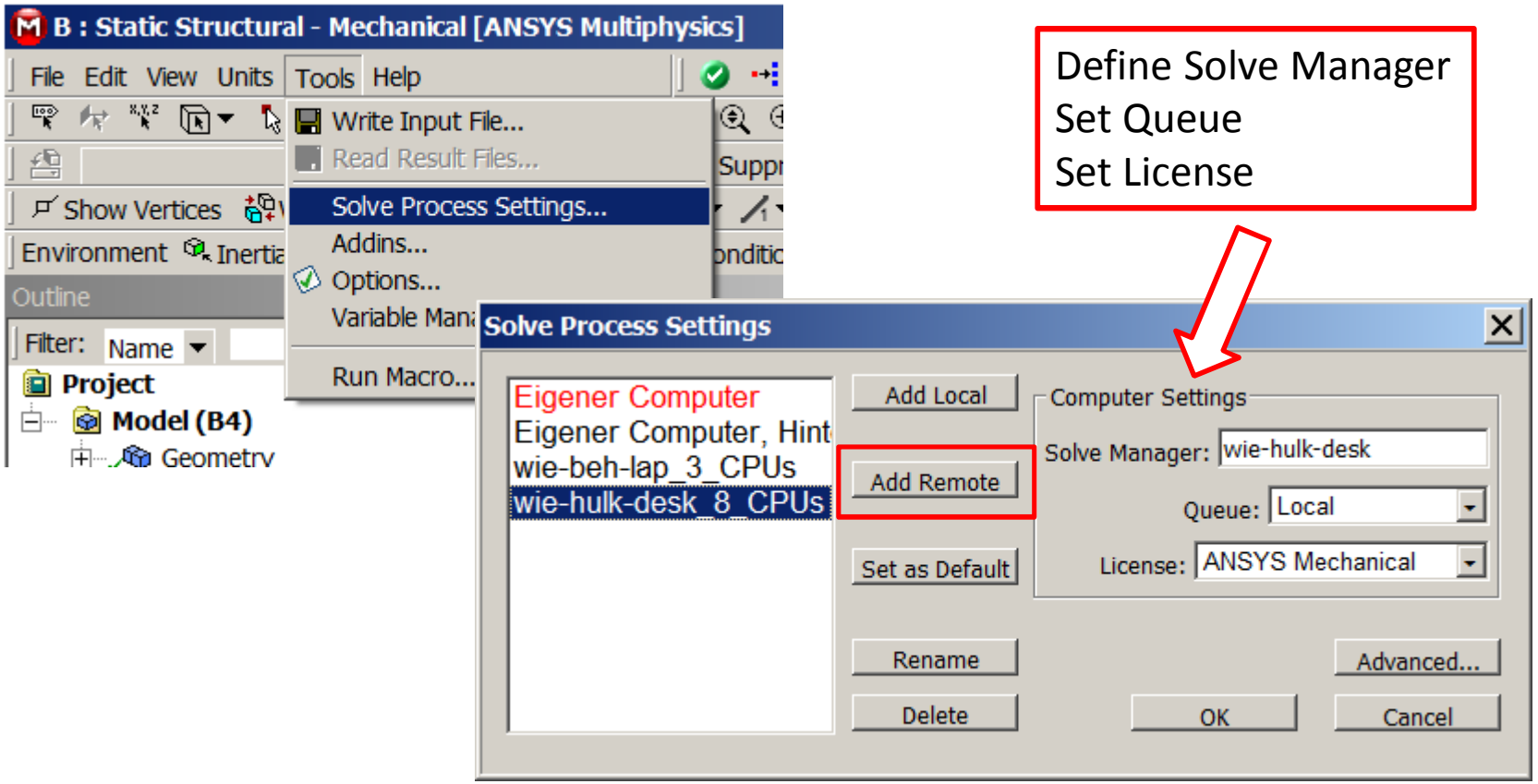
The following ports must be open for Communication between RSM components

ANSYS 14: 8140 and 9140

ANSYS 14.5: 8145 and 9145

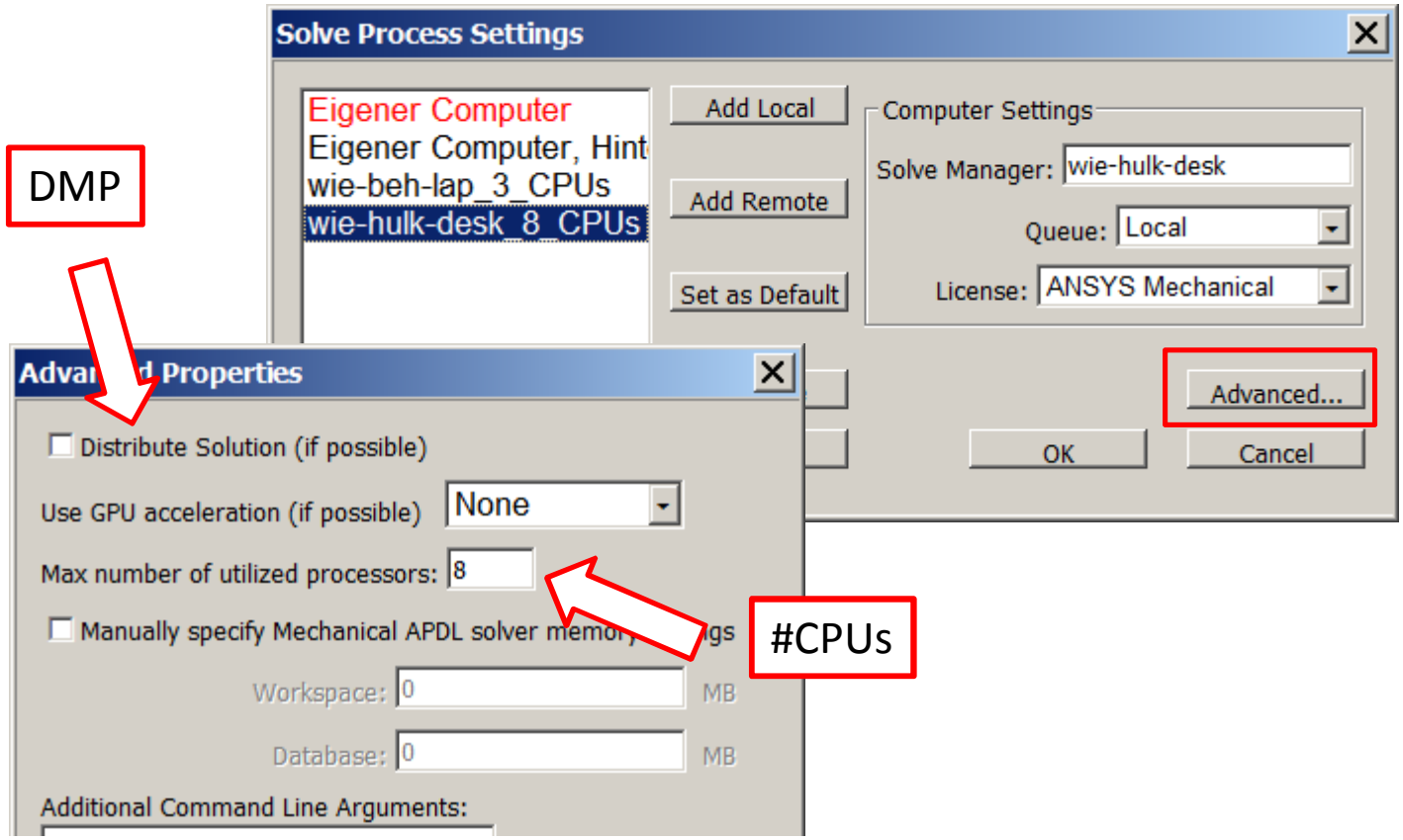
How to Set up HPC ï Solver Handler

Å Setup solver handler



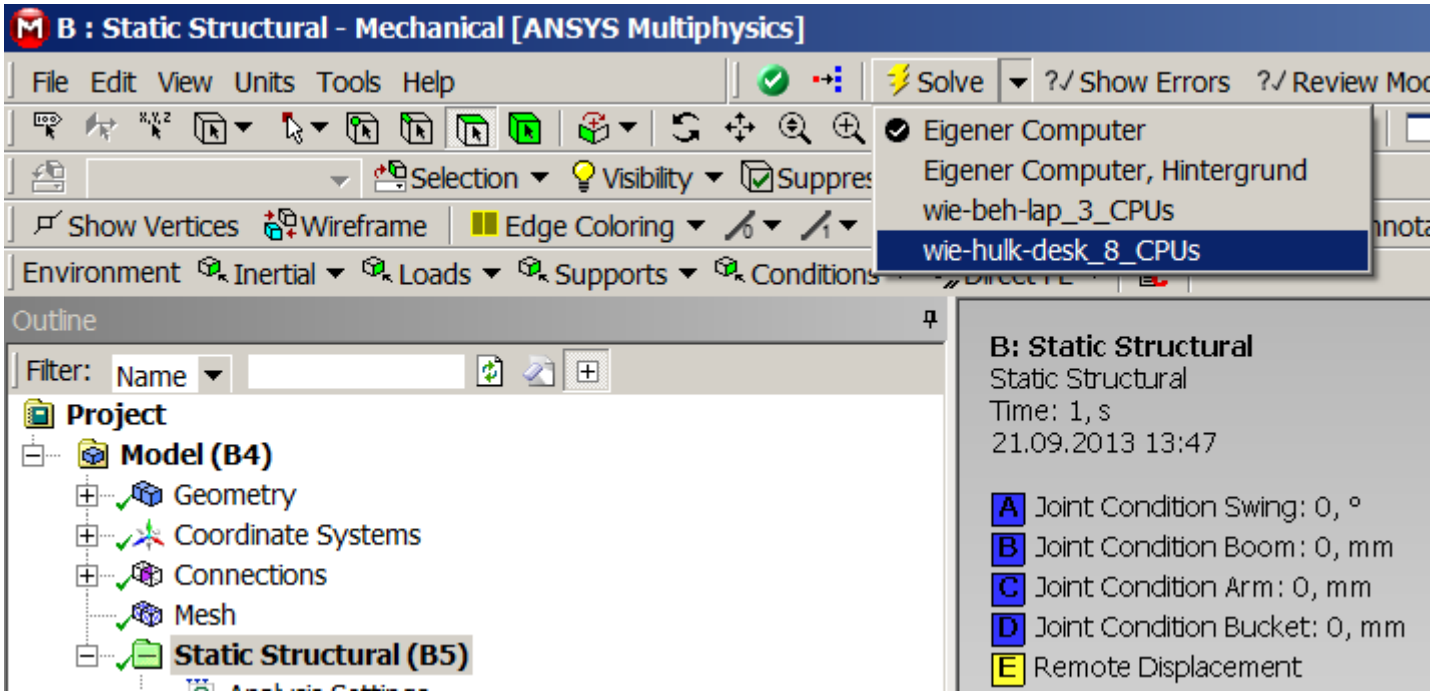
How to Set up HPC ï Solver Handler

Å Setup solver handler



How to Set up HPC ï Solver Handler

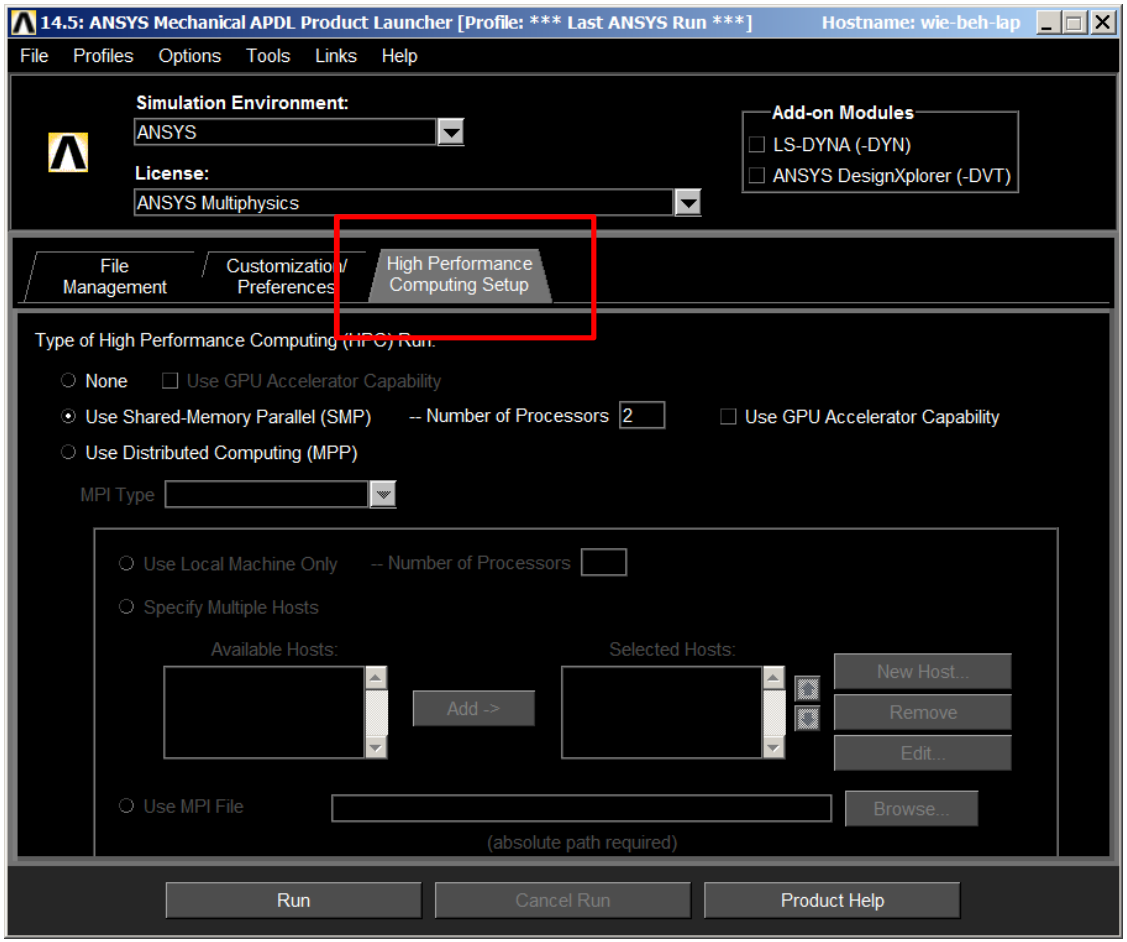
Å Use the desired solve handler



The solver handler are saved in the file “solvehandlers.xml” which can be located in %appdata%\ansys\programversion.

How to Set up HPC ï Mechanical APDL

Å Start ANSYS product launcher

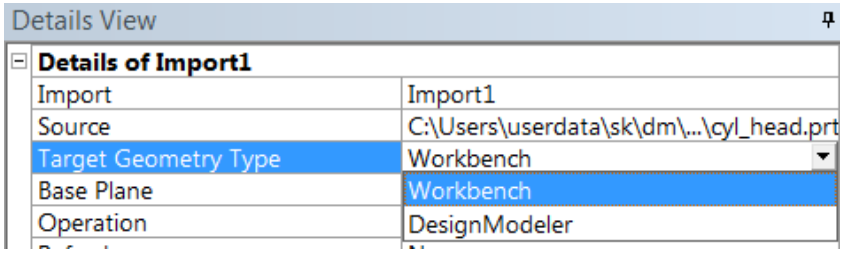


Handling of Large Models ï CAD Import

- Import/Attach feature now supports two options for target geometry type:
  - DesignModeler
    - Full conversion to DMôs internal representation (Parasolid)
    - Traditional behavior
  - Workbench
    - Light-weight B-rep
    - Faster import from external CAD system into DM

> DM automatically converts entities during modeling, as needed

> Manual conversion with the new ôConversionô Feature



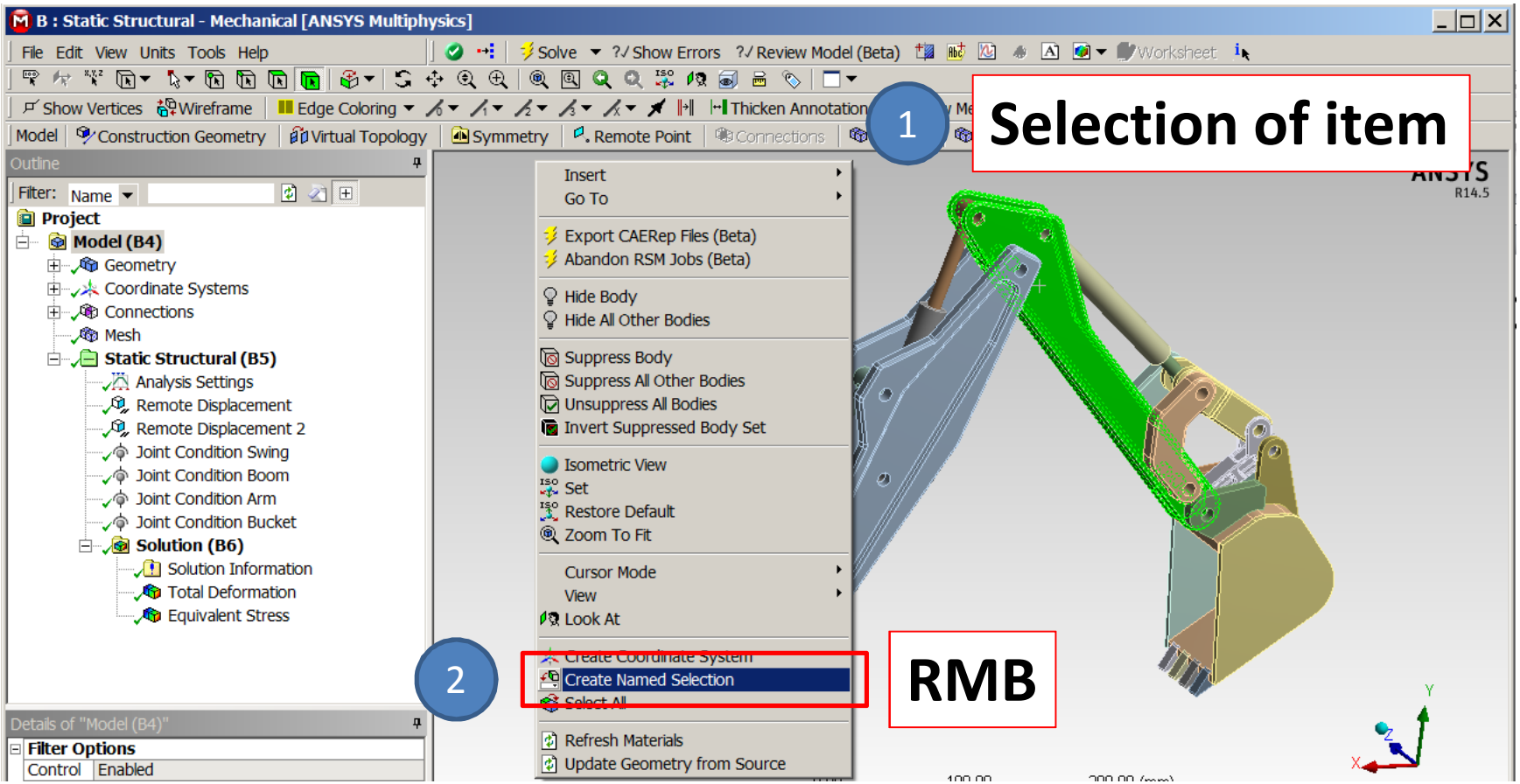
Import Time in 14.0	Import Time in 14.5 (WB geometry type)
110 minutes	5 Minutes

Handling of large models ï Named selections

- Named selections can used to:
  - Filter items
  - Group items
  - Convert items
- This is of interest for:
  - Programming macros
  - Fast selection of similar items used for Pre- and Postprocessing
  - Easier navigation through the model

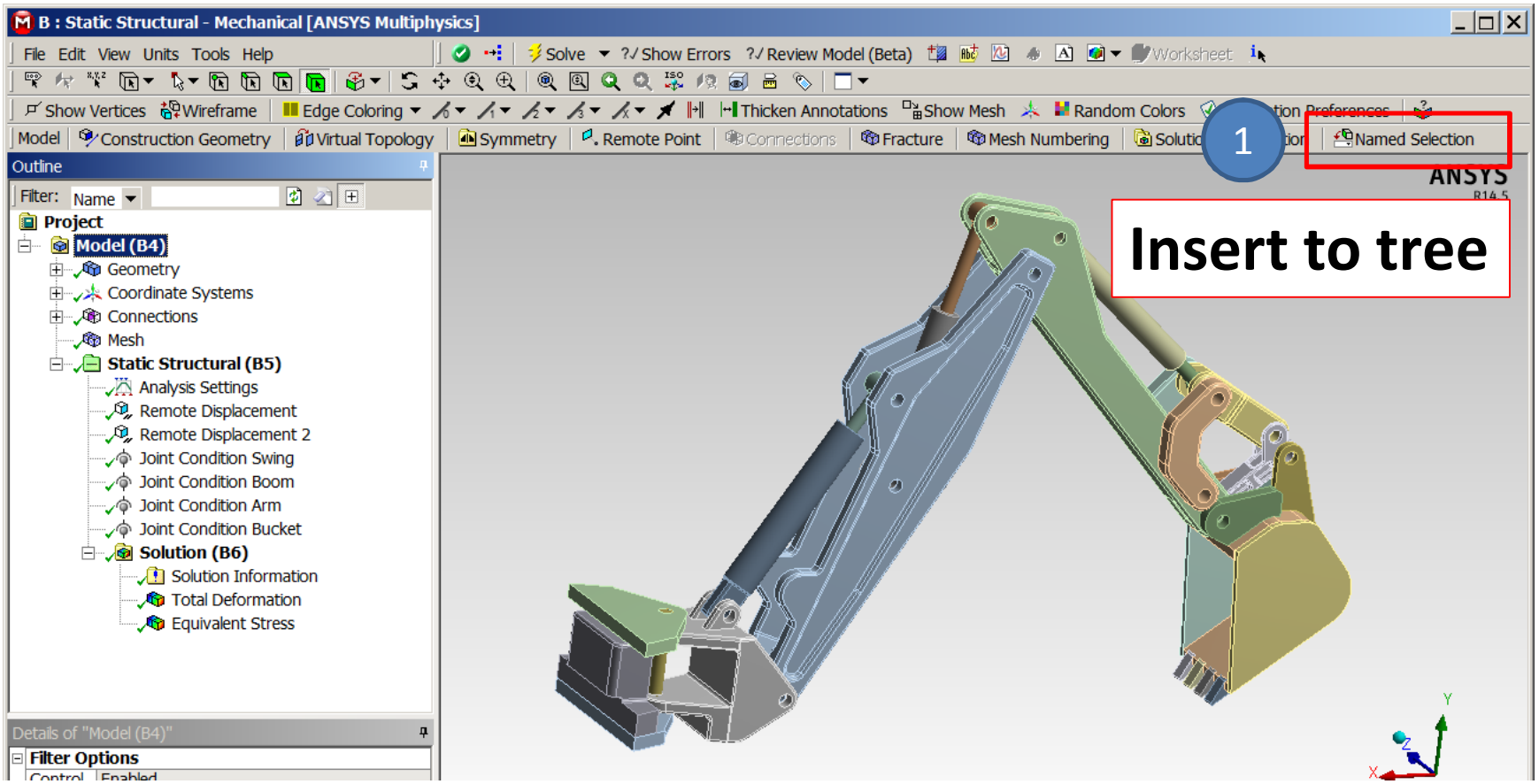
Handling of Large Models ï Named Selections

Å How to insert a Named Selection item #1



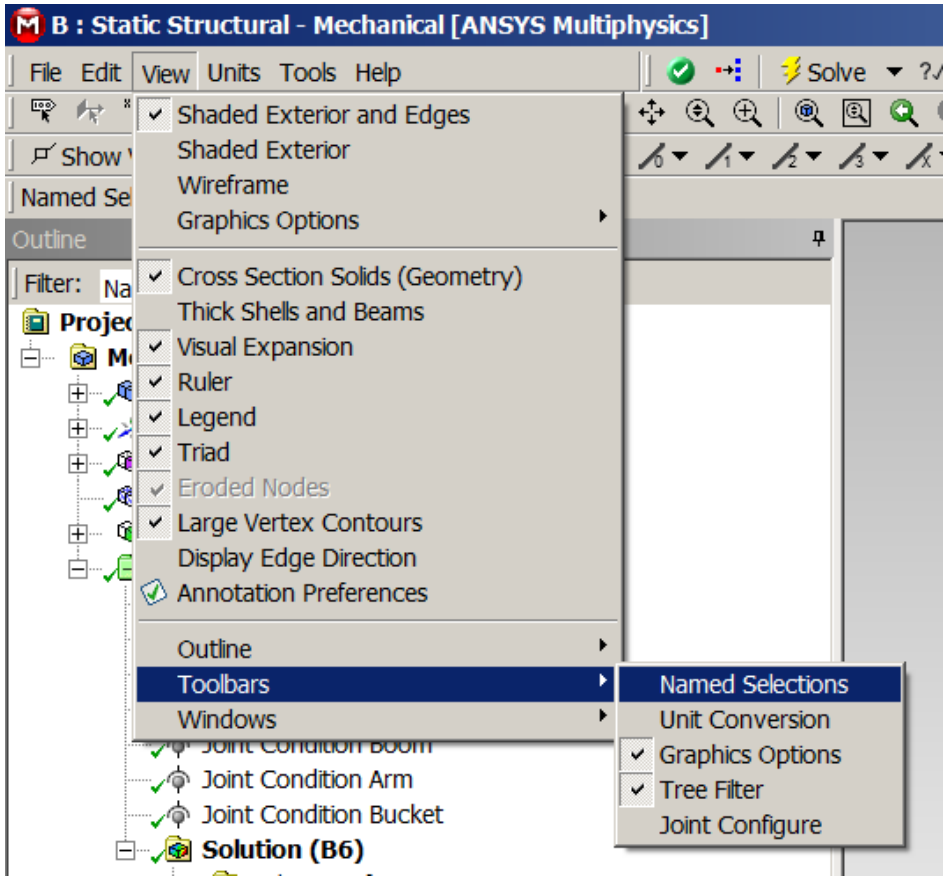
Handling of Large Models ï Named Selections

Å How to insert a Named Selection item #2



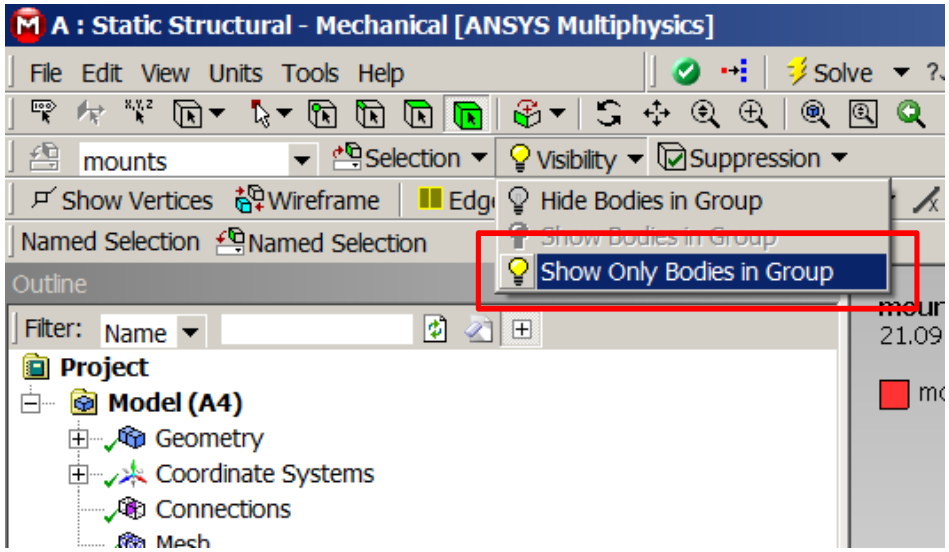
Handling of Large Models ï Named Selections

- Insert Toolbar for fast selection



Handling of Large Models ï Named Selections

- Working with the toolbar



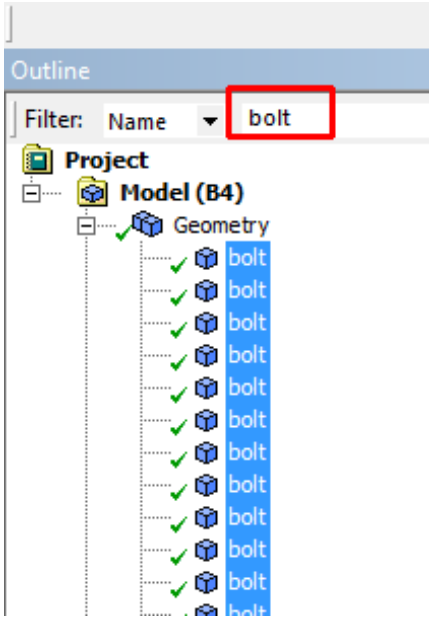
→ **Example: excavator.*wbpz; helicopter.wbpz***

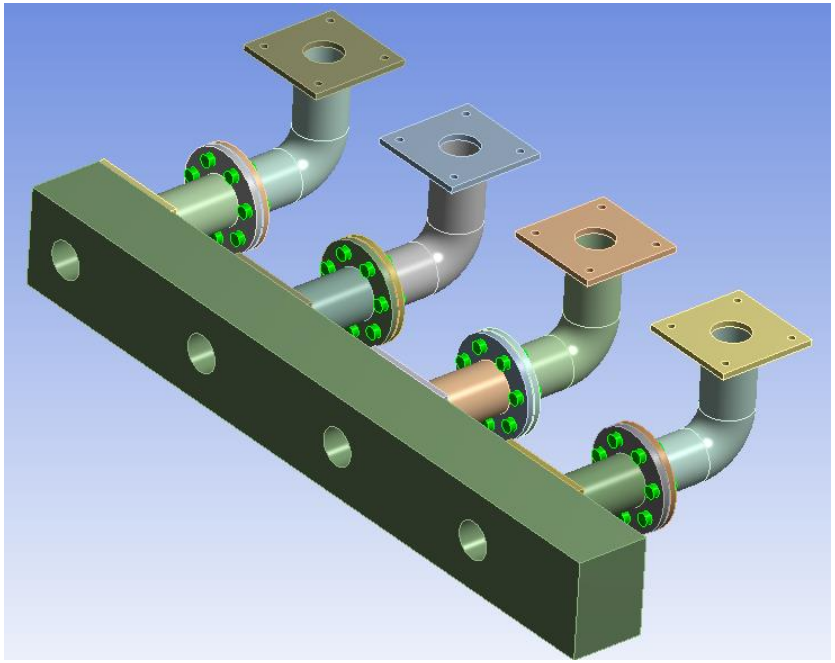
Handling of Large Models ï Tree Filter and Tags

- Tree Filter:
  - Users want the ability to control the amount of data shown in the Mechanical tree view.
  - The Tree Filter allows users to show only those objects which match some search terms.
  - The filter searches on *object name* or on *object tags*.

Handling of Large Models ï Tree Filter and Tags

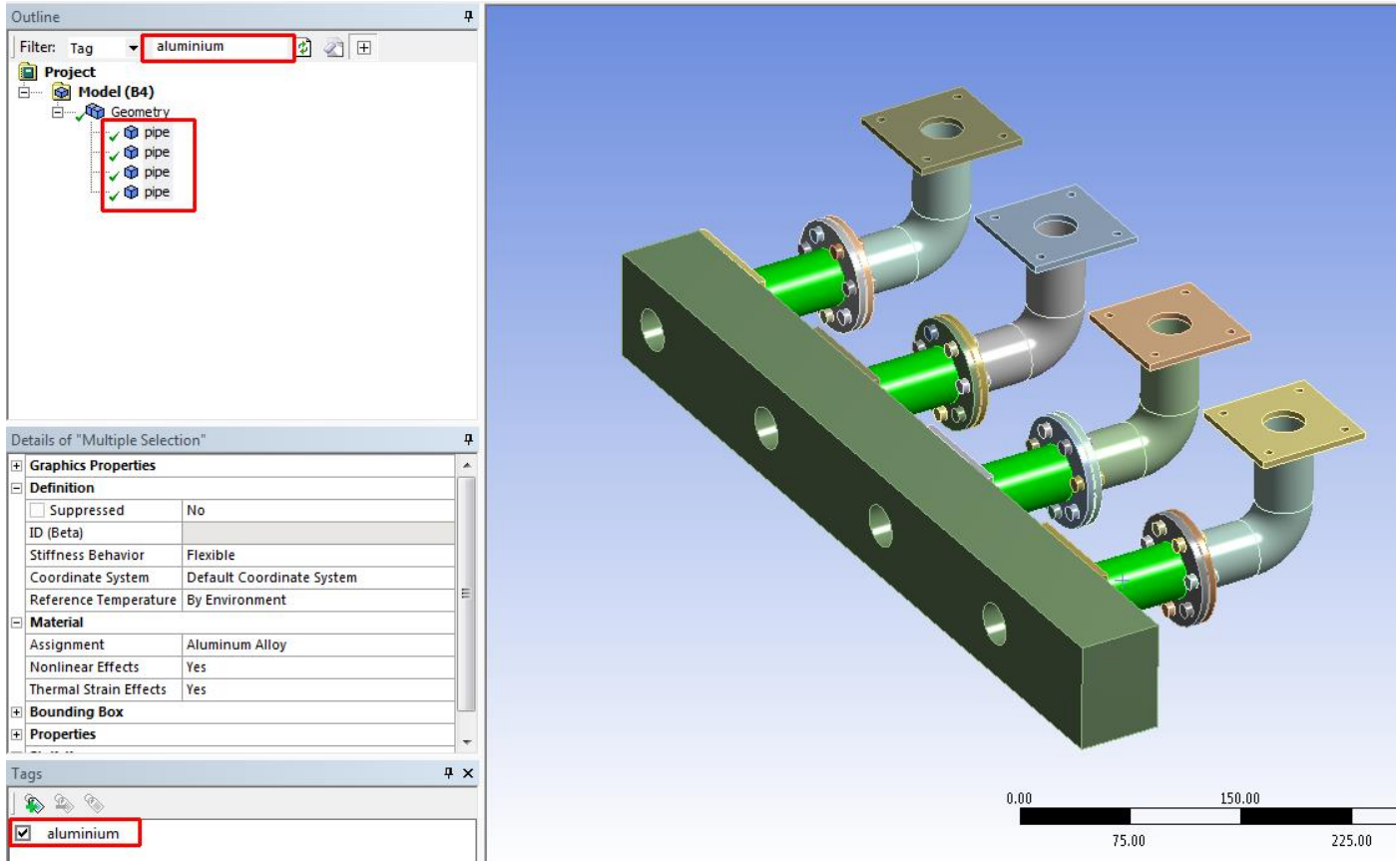
Å Entering a search term, e.g. ñbolt,òand hitting Enter filters the tree to show only those objects with names matching ñbolt.ò





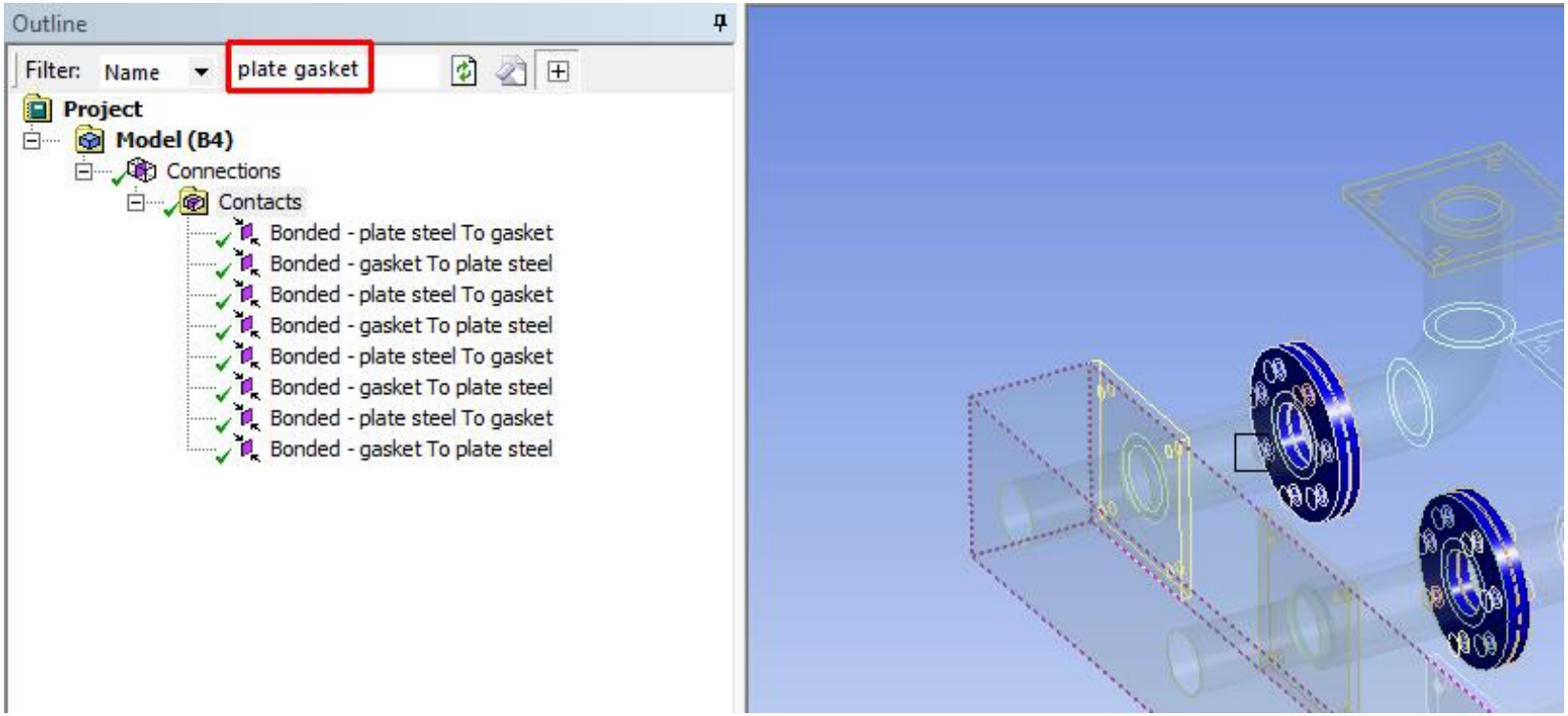
Handling of Large Models ï Tree Filter and Tags

- A similar search can be performed on object tags by selecting ñTagsòfrom the drop-down menu.



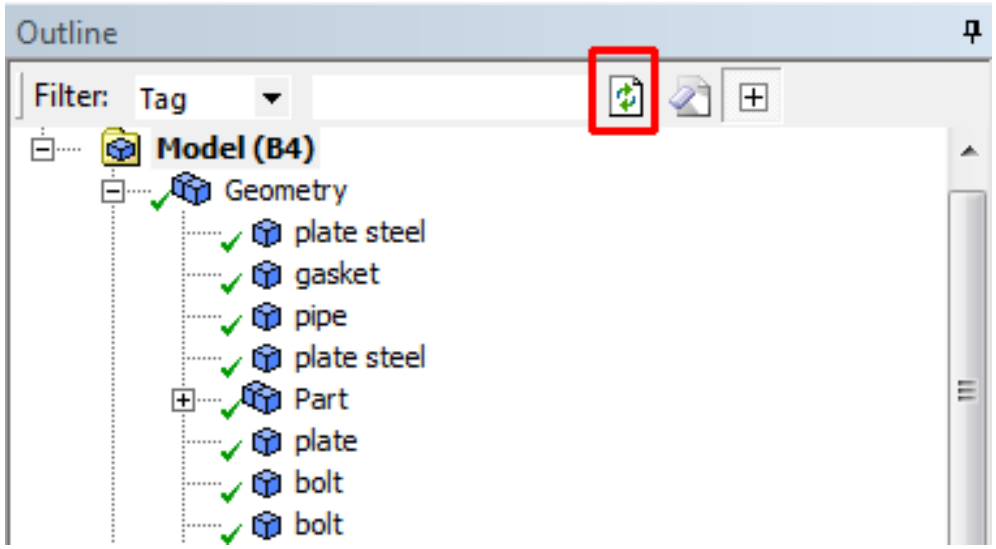
Handling of Large Models ï Tree Filter and Tags

Å Multiple search terms are supported, so all objects with ñplateòand ñgasketòcan be found with ñgasket plate ò (case sensitive).



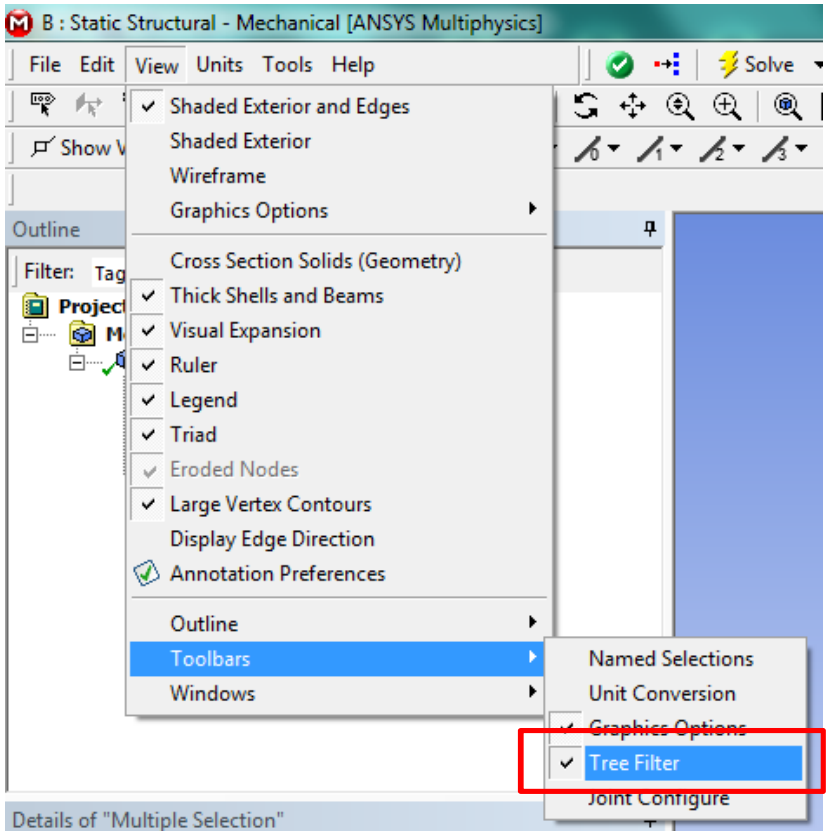
Handling of Large Models ï Tree Filter and Tags

- When filtering is in effect, any object that is added, removed, or renamed will not be affected until filtering is manually refreshed.



Handling of Large Models ï Tree Filter and Tags

Å The Tree Filter can be turned off under View → Toolbars (Mechanical recalls last visibility setting on startup).



→ **Example: *tree_filter.wbpj***

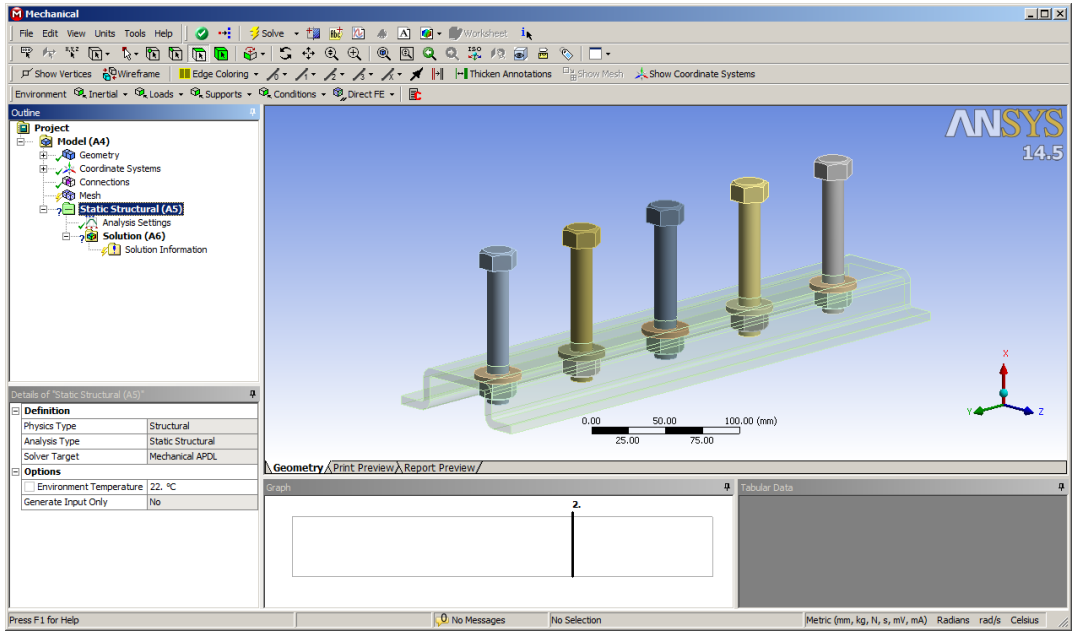
Handling of Large Models ï Object Generator

- Object Generator
  - ï Users want the ability to make multiple copies of objects, scoping each to different geometry.
  - ï The Object Generator allows users to use an existing object as a template for replication.
  - ï Almost any tree object that supports ñDuplicateò can be used as a template.

Handling of Large Models ï Object Generator

Å Typical Application:

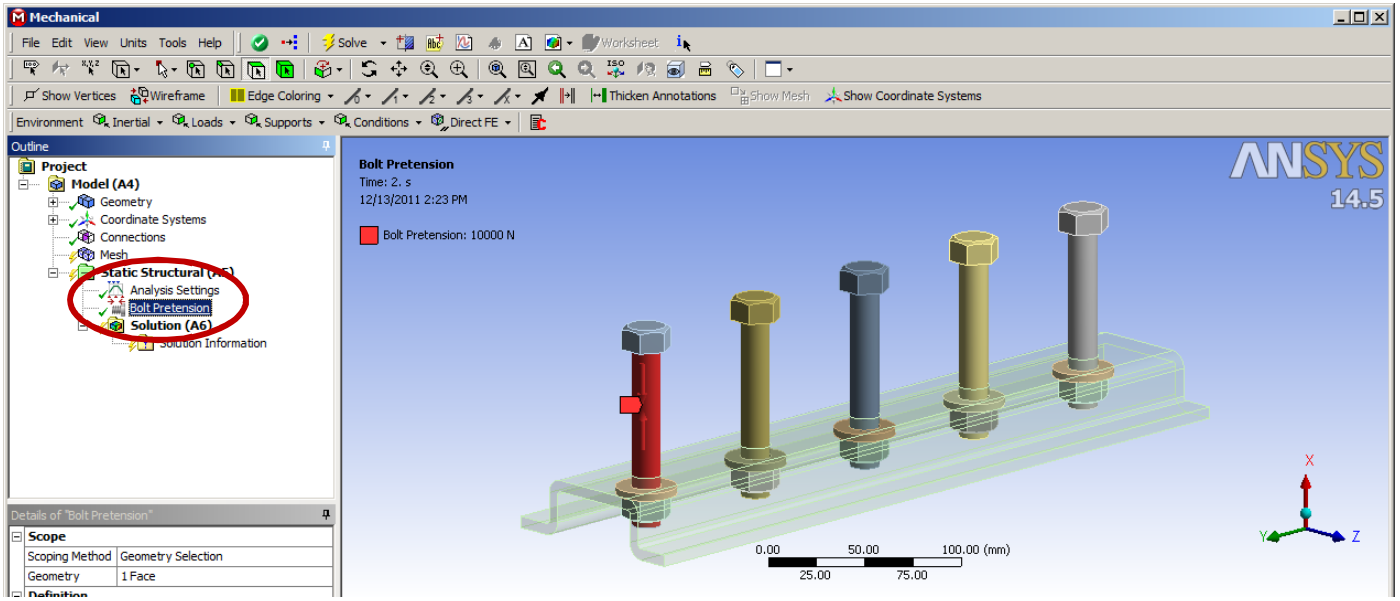
ï The user has many bolts in a model and wants to apply a bolt pretension load to each bolt



Handling of Large Models ï Object Generator

Å Step 1:

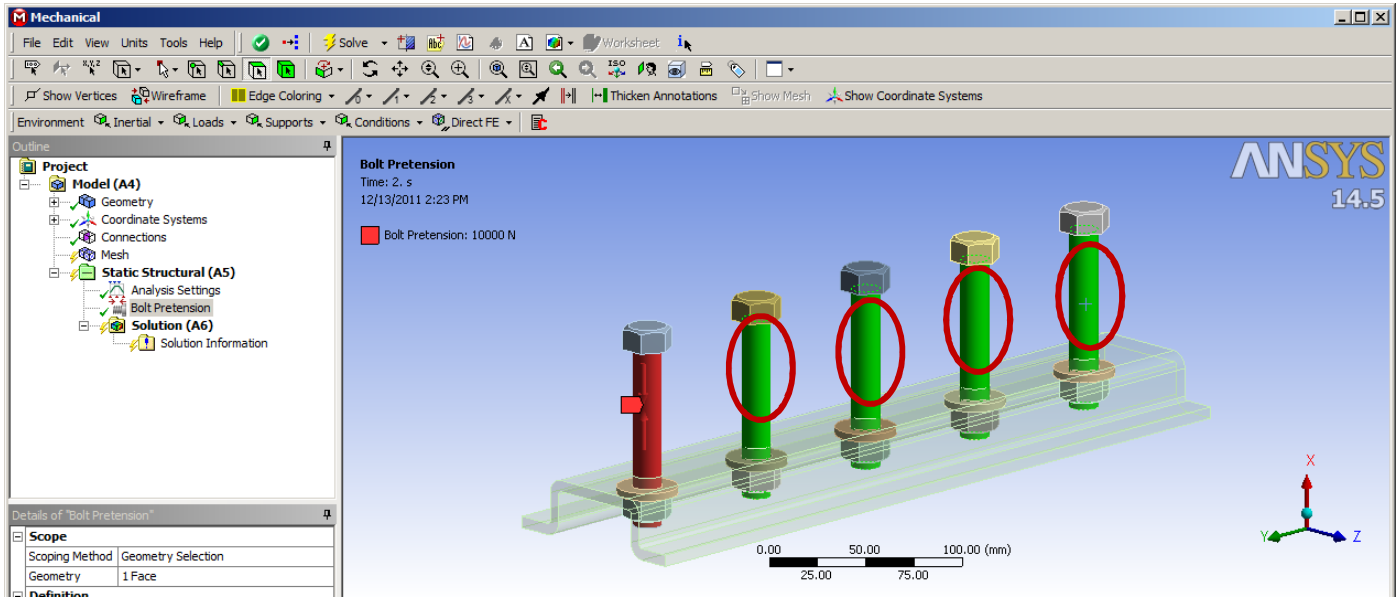
ï Define the tree object to be copied (optionally define Details).



Handling of Large Models ï Object Generator

Å Step 2:

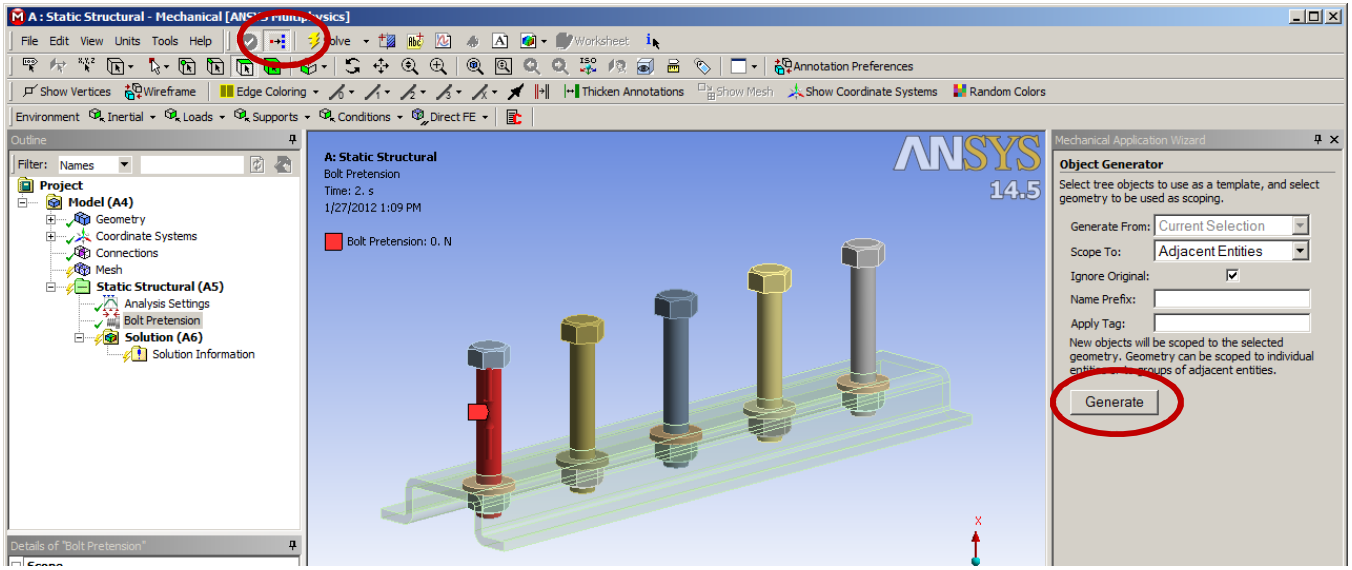
ï Select the geometry to which the tree object should be copied.



Handling of Large Models ï Object Generator

Å Step 3:

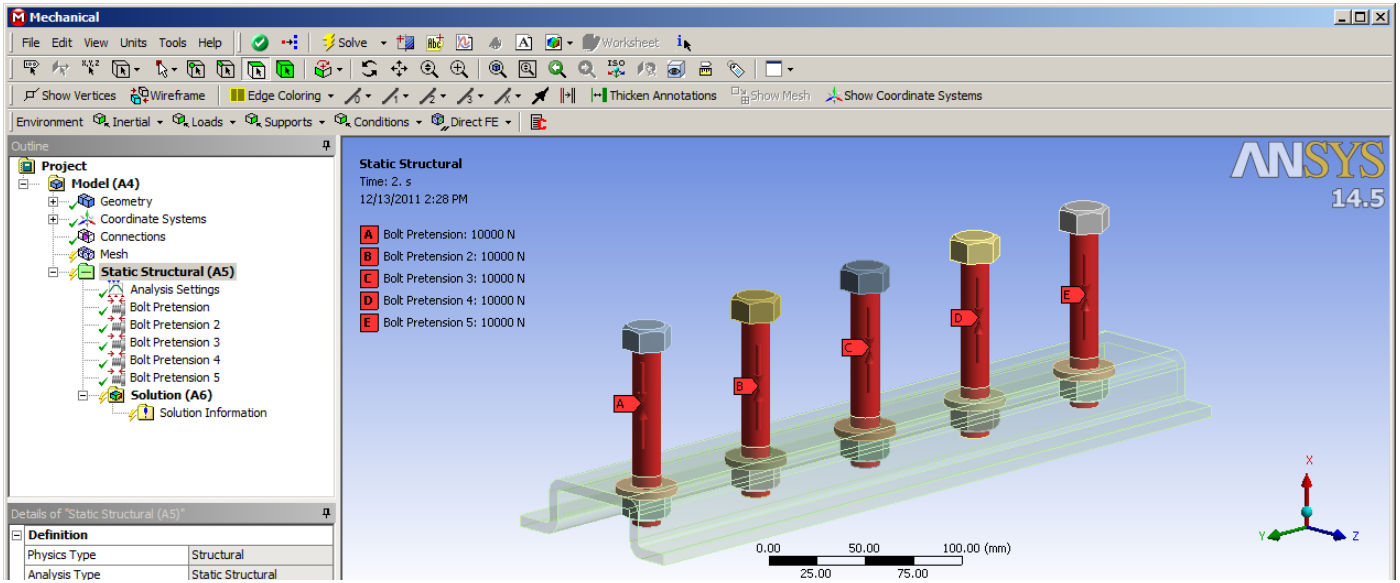
ï Open the Object Generator and click ñGenerateò



Handling of Large Models ï Object Generator

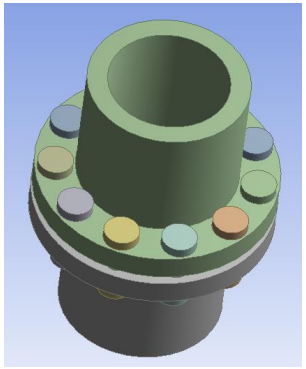
Å Result:

- ï The original load was copied to all selected geometry. *All details* from the original template object are maintained.



Handling of Large Models ï Object Generator

- Task:
  - ï Connection with many bolts, axial forces in the bolts needed



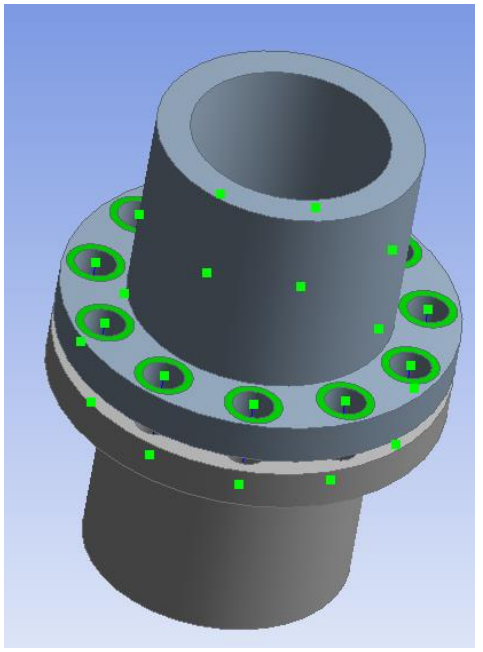
- Idea:
  - ï Use Beams for easy postprocessing
- Drawback:
  - ï Multiple preprocessing actions needed, 1 bolt pretension per bolt and 2 connections for each of the beams
- Solution
  - ï Use object generator for convenience.

→ **Example: *object_generator.wbpz***

Handling of Large Models ï Object Generator

Å Preparation:

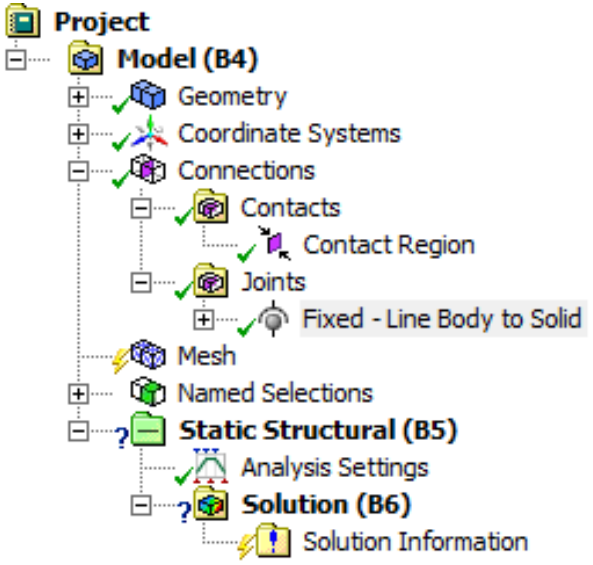
- ï We need **named selections** for the object generator. If the pattern operation is done in **Design Modeler** you can define the component before creating the pattern and use **propagate selection**, so you only need to click one face.

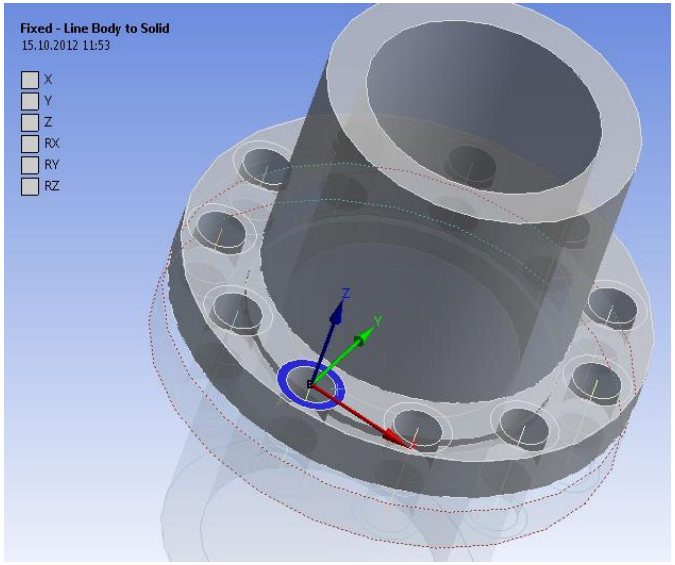


Details of Koppelflaeche	
Named Selection	Koppelflaeche
Geometry	22 Faces
Propagate Selection	Yes
Export Selection	Yes

Handling of Large Models ï Object Generator

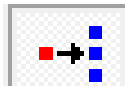
- In ANSYS Mechanical
  - Define the object you want to copy multiple times.

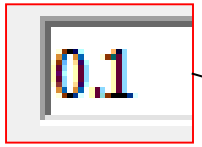


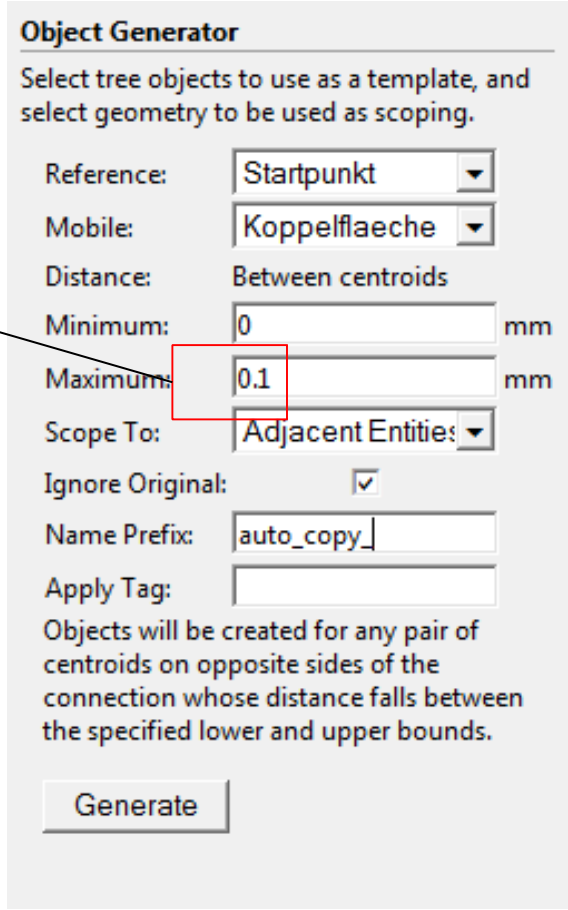


Handling of Large Models ï Object Generator

- In ANSYS Mechanical
  - Activate the object generator.
  - Assign the named selections
  - Define a tolerance
  - Specify a prefix, so you can easily see the generated connections
  - As a result you receive multiple joints.

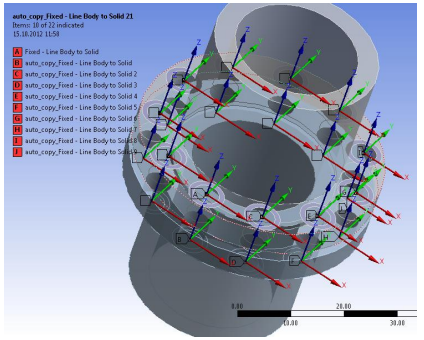






Handling of Large Models ï Object Generator

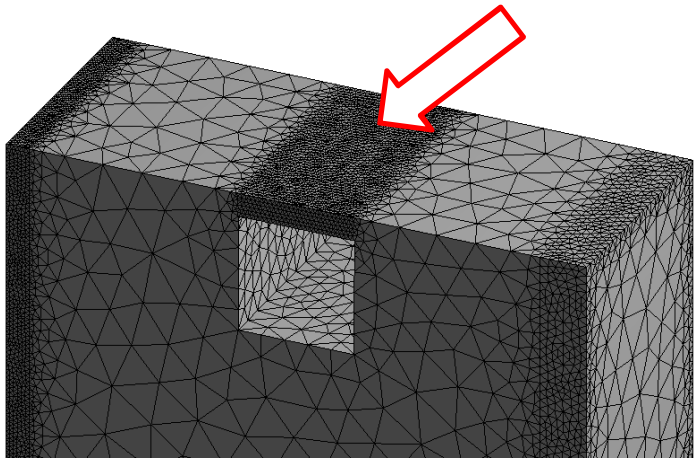
- Now we can repeat the process with the bolt pretension.
  - Define first bolt pretension
  - Use named selections with all line bodies (tolerance not needed, because there is a clear relation)
  - Generate pretension for all 11 bolts.

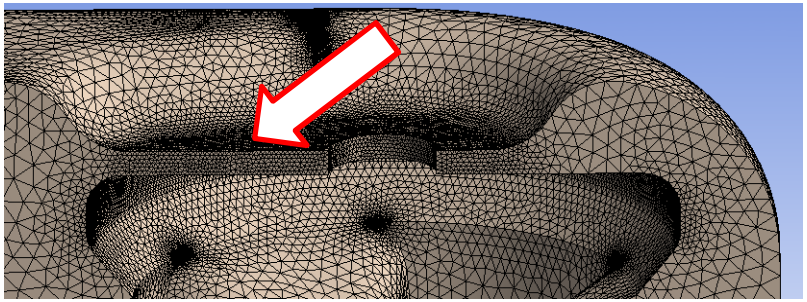


Part II

Mesh Controls for Large Models - Curvature and Proximity

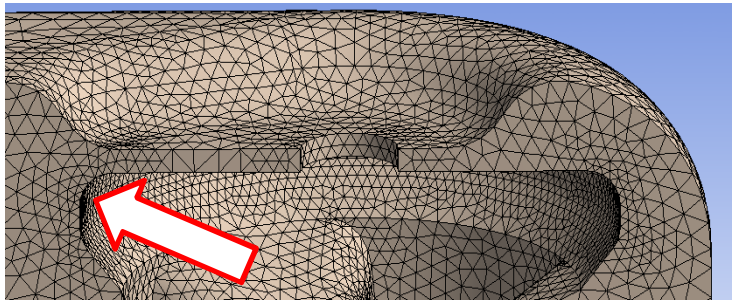
- The proximity size function allows you to specify the minimum number of element layers created in regions that constitute ‘gaps’.

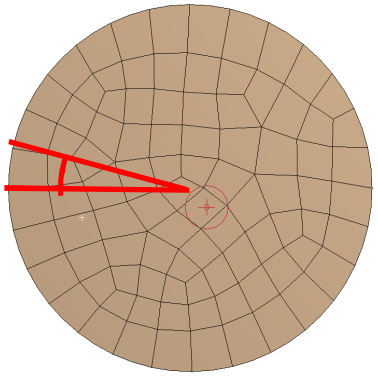




Mesh Controls for Large Models - Curvature and Proximity

- The curvature size function examines curvature on edges and faces and computes element sizes on these entities such that the size will not violate the **maximum size** or the **curvature normal angle**.





curvature normal angle

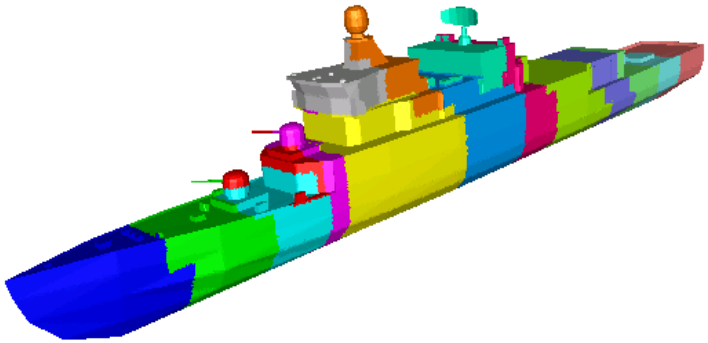
Mesh Controls for Large Models - Curvature and Proximity

- Important: using curvature and/or proximity usually results in very big models because small details are densely meshed.

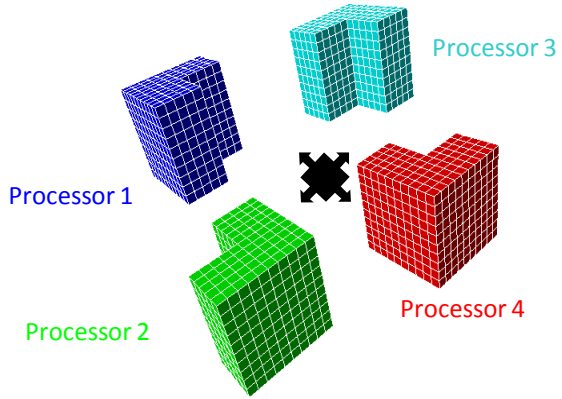
  -> HPC might be important

How to Cut Analysis Time – Contact Settings

- The key concept of HPC is domain decomposition
  - Break problem into *N* pieces (domains)
  - "Solve" the global problem independently within each domain
  - Communicate information across the boundaries as necessary



Source: IBM



Source: ANSYS

Source: IBM

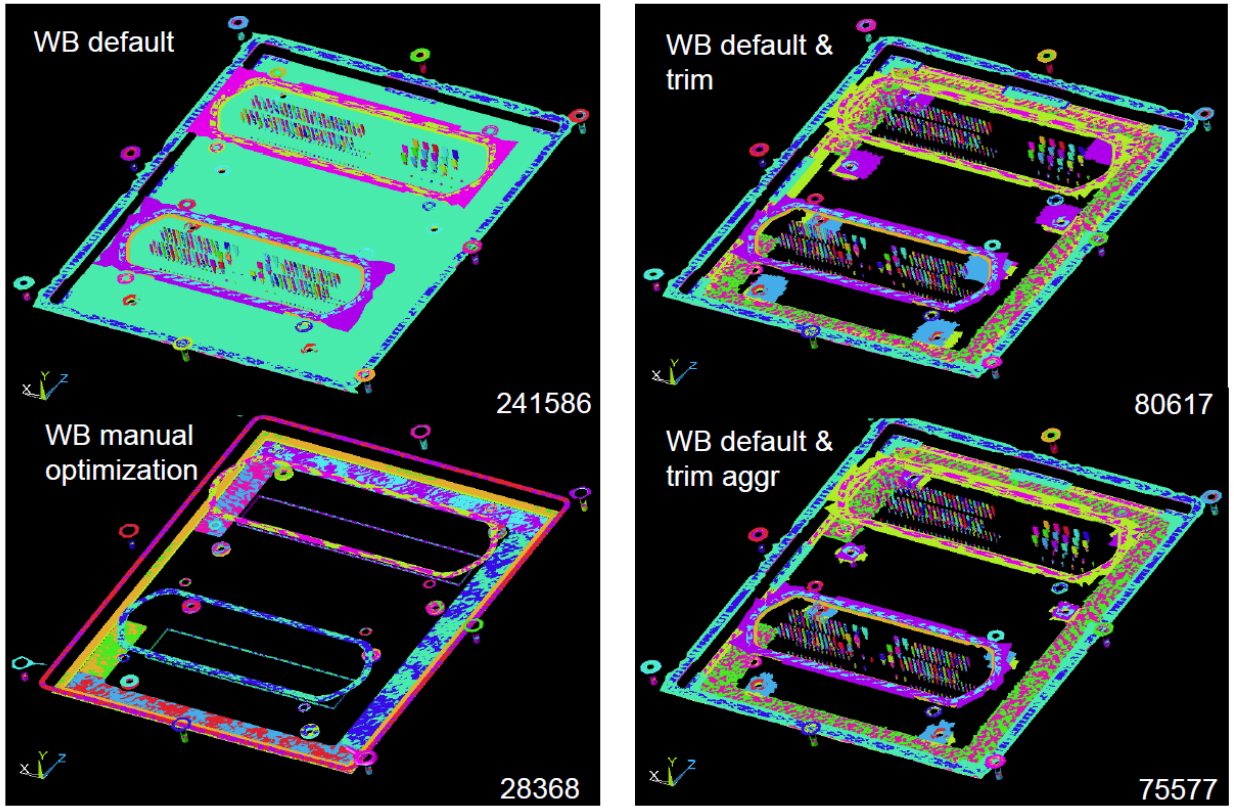
How to Cut Analysis Time – Contact Settings

- When using contacts each of the contact pairs has to be analyzed in the same domain.
- Large contact areas slow down the analysis.
- Help: trim contact areas
- APDL command: **CNCHECK,TRIM**

How to Cut Analysis Time – Contact Settings

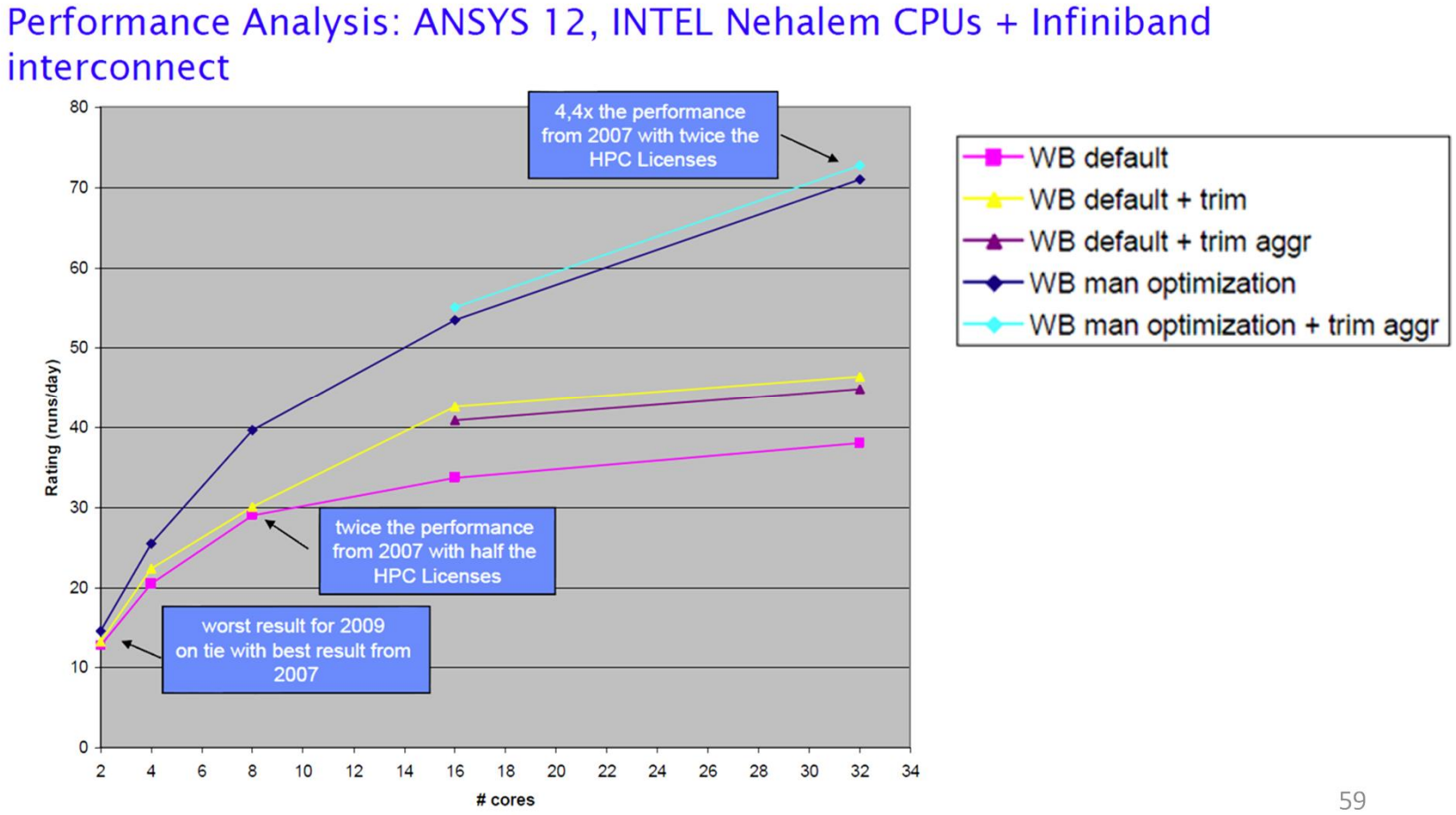
Å Example of socket with non-linear contacts

Meshing results (contact elements only)



How to Cut Analysis Time – Contact Settings

Å Example of socket with non-linear contacts



How to Cut Analysis Time – Solver Settings

- D-ANSYS (DMP) vs. ANSYS (SMP)
  - The entire SOLVE phase is parallel: including element matrix generation, linear equation solver, and element results calculation
  - More of the analysis is performed in parallel
  - Better scaling than SMP, between 2X to 7X speedup on 2 to 16 processors!
  - Memory usage also scales in most cases.
  - Disk (I/O) usage also scales. Separate I/O files are managed on each processor

How to Cut Analysis Time – Solver Settings

- Sparse Solver (Direct Solver)
  - Efficient when the resulting stiffness matrix is **unsymmetric** (e.g. irreversible operations like contact with friction, plasticity)
  - Efficient when the resulting stiffness matrix is **ill conditioned** (e.g. weak springs, numerous contacts, plasticity with K->0, skewed elements)
  - Can be used in contact analysis with **Lagrange Formulation**
  - Can be used for **mixed u-P element Formulation** (hyperelasticity, plasticity)

How to Cut Analysis Time – Solver Settings

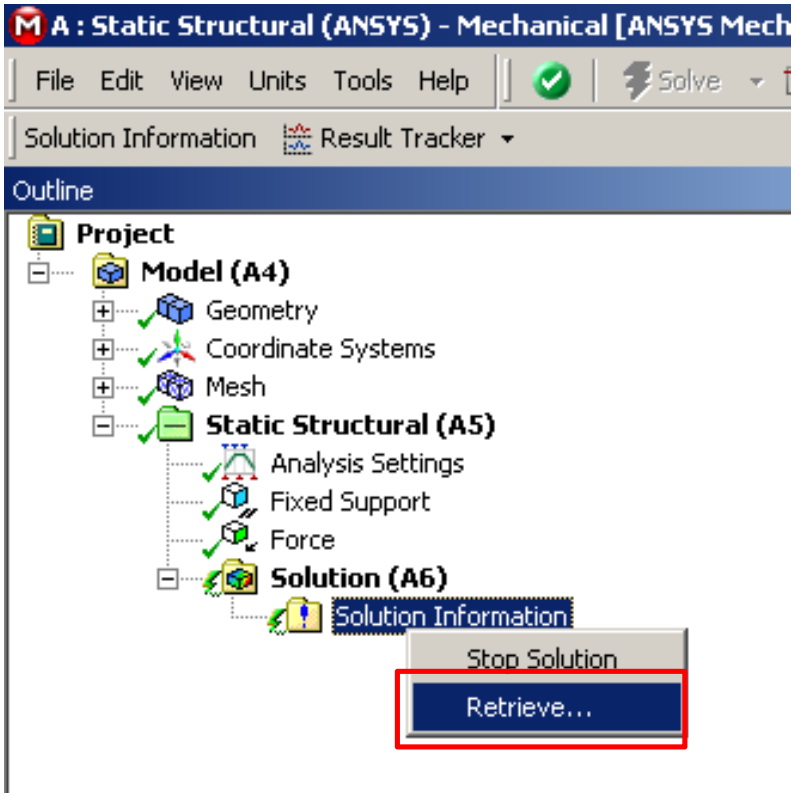
- PCG (Iterative Solver)
  - Efficient with **very fine** meshes of solid elements
  - Working with symmetric matrices only
  - Takes less RAM than Sparse Solver
  - Swaps between RAM and Disk -> SSD-Disks no problem
  - When using the command PCGOPT it can be used when **joints** (MPC184 elements) are present in the model

How to Cut Analysis Time – Solver Settings

- Solver options that save analysis time
  - **`bcsoption,,incore`** for Sparse Solver
  - **`dspoption,,incore,,,,performance`** for DSparse Solver
  - **`pcgopt,lev_diff`**: settings for level of difficulty
    - when using up to 4 cores stick with AUTO
    - When using 8 or more cores then:
      - If AUTO picks a *Lev_Diff* value = 1, stick with that
      - If AUTO picks a *Lev_Diff* value ≥ 2, consider lowering *Lev_Diff* value by 1

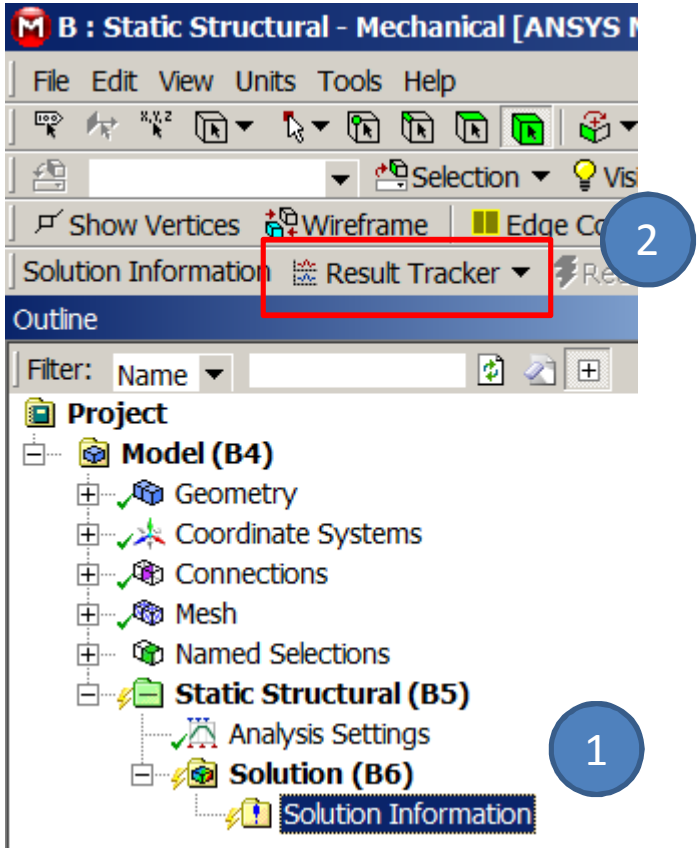
Evaluation of Results – The Result Tracker

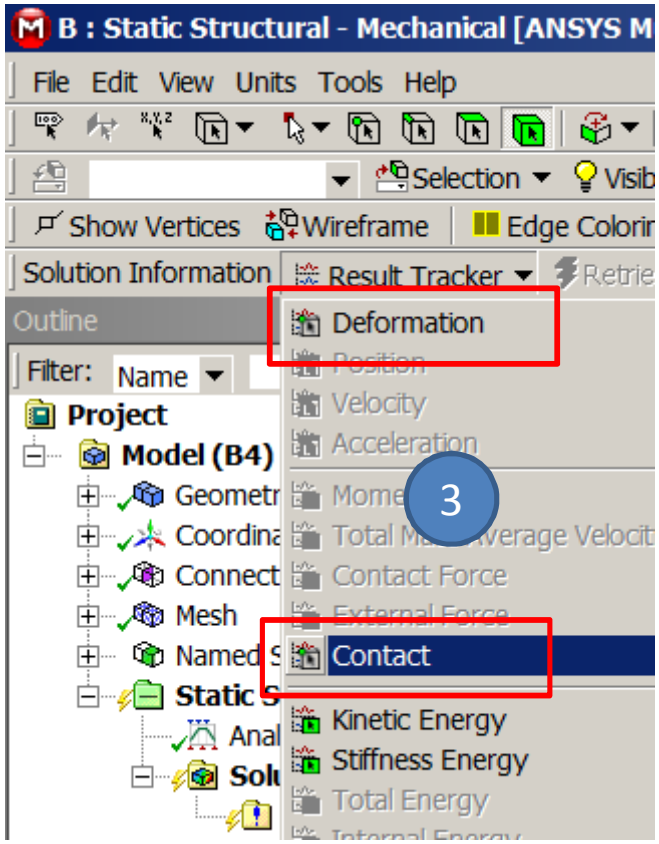
Å Check solution status during run using RSM



Evaluation of Results – The Result Tracker

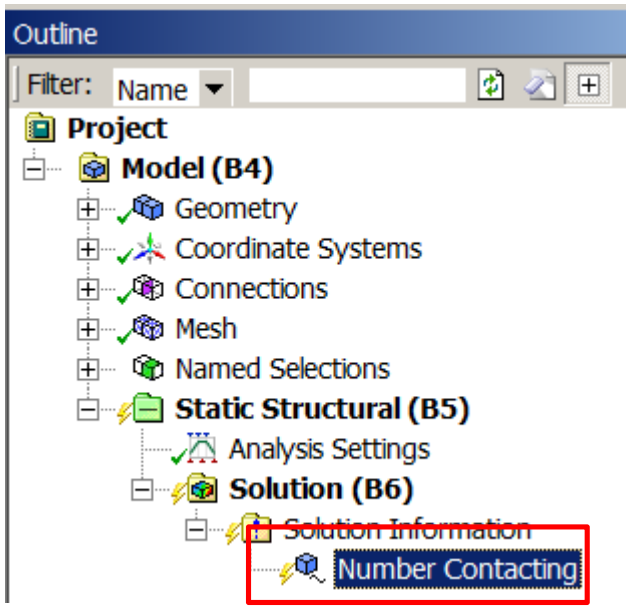
Å Insert result item you like to track during solution – **has to be done before analysis**

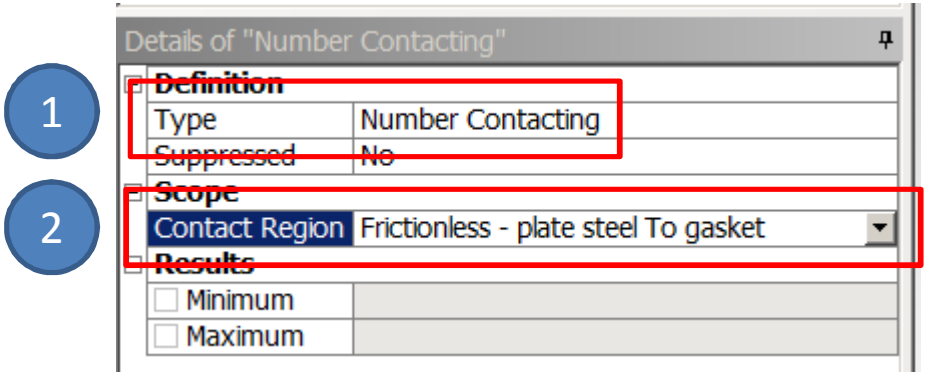




Evaluation of Results – The Result Tracker

Å Define Details



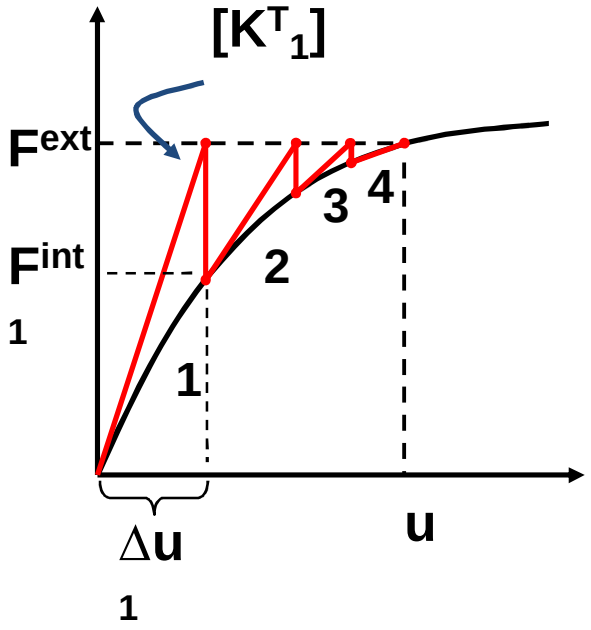


Evaluation of Results - Newton Raphson Residuals and RSM

Å What are Newton Raphson Residuals

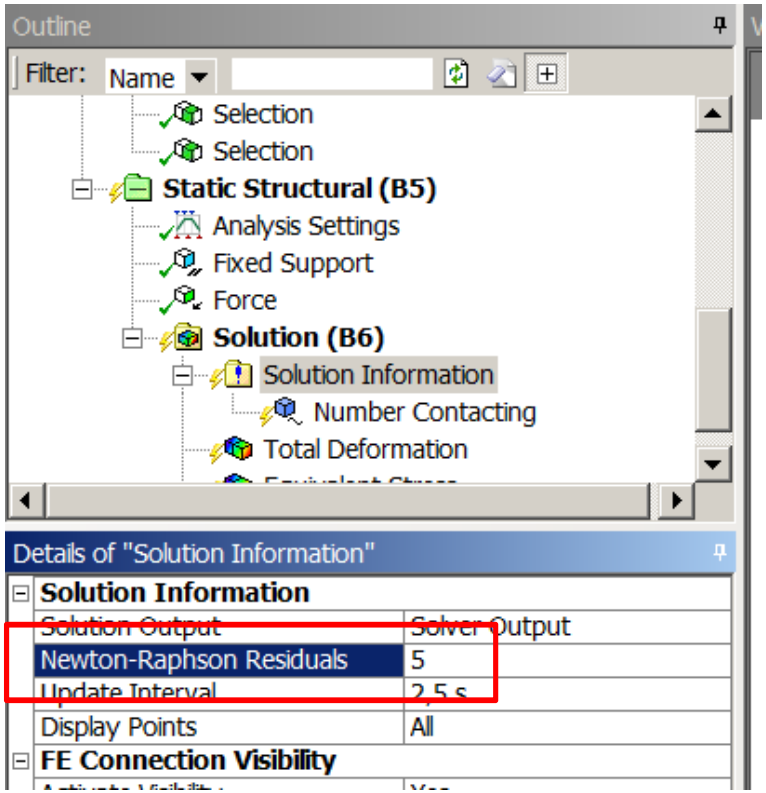
$$[K^T]\{\Delta u\} = \{F^{ext}\} - \{F^{int}\}$$

$[K^T]$ = Tangential stiffness matrix
$\{\Delta u\}$ = Vector of displacement increments
$\{F^{ext}\}$ = Vector of external loads
$\{F^{int}\}$ = Vector of internal loads



Evaluation of Results - Newton Raphson Residuals and RSM

Å Choose number of iterations for which you like to see the Newton Raphson Residuals



Evaluation of Results - Newton Raphson Residuals and RSM

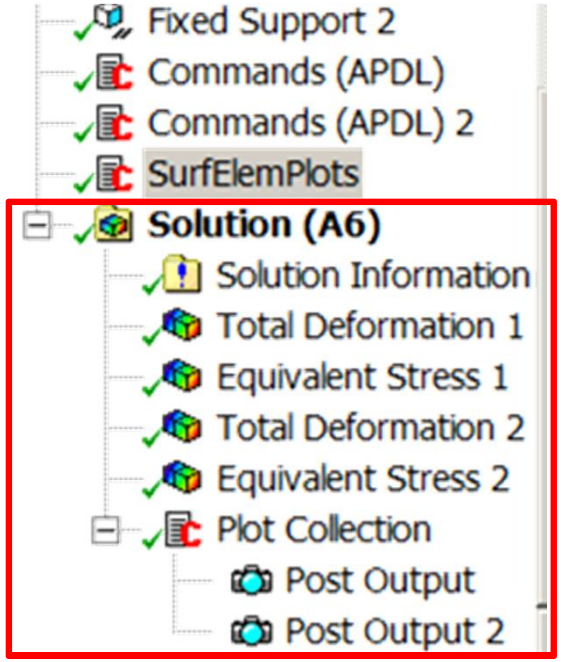
- In order to evaluate the Newton Raphson Residuals in case an analysis is not converging do the following:
- Open the file:
  - **C:\Program Files\ANSYS Inc\v145\RSM\Config\xml\Ansys_Generic.xml**
- Add the line:
  - **<file type="binary" special="SolutionInformation">file.nr*</file>**

Evaluation of Results - Newton Raphson Residuals and RSM

```
<?xml version="1.0"?>
<jobTemplate>
        <script>GenericJobCode.xml</script>
        <debug>FALSE</debug>
        <cleanup>TRUE</cleanup>
        <inputs>
    <file type="ascii" special="cancel">file.abt</file>
  </inputs>
        <outputs>
    <!--<file type="ascii">*.out</file>  Use this to get additional *.out files -->
    <file type="ascii" special="SolutionInformation">solve.out</file>
    <file type="ascii" special="SolutionInformation">file.gst</file>
                <file type="ascii" special="SolutionInformation">file.nlh</file>
    <file type="ascii" special="SolutionInformation">file0.gst</file>
    <file type="ascii" special="SolutionInformation">file0.nlh</file>
    <file type="binary" special="PostDuringSolve">file.rcn</file>
    <file type="ascii" special="PostDuringSolve">file0.nlh</file>
    <file type="ascii" special="cancel">file*.err</file>
    <file type="ascii" special="cancel">solve.out</file>
    <file type="binary" special="SolutionInformation">file.nr*</file>
  </outputs>
</jobTemplate>
```

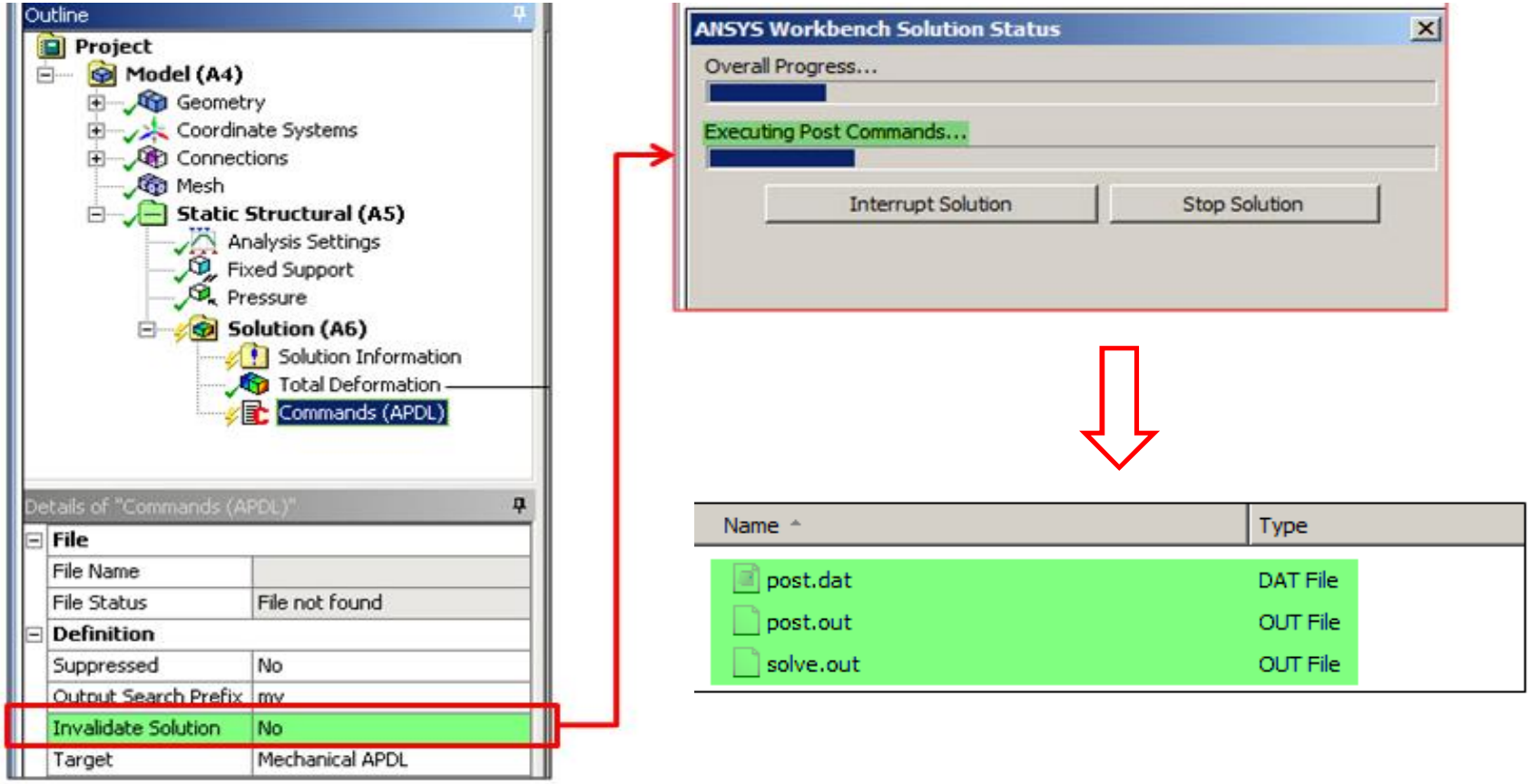
Evaluation of Results – Postprocessing Command Snippets

- During Postprocessing you can use your own APDL routines to list items, plot results, and do your own calculations.



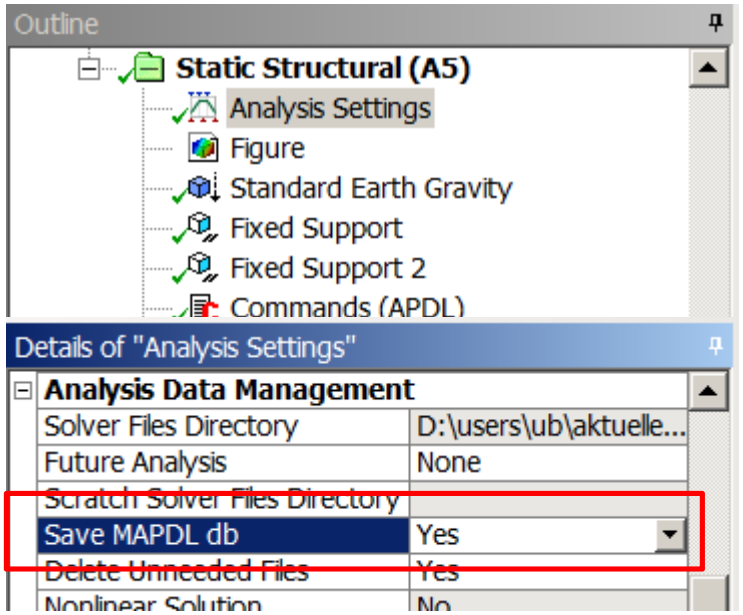
Evaluation of Results – Postprocessing Command Snippets

Å Check setting “Invalidate Solution”



Evaluation of Results – Postprocessing Command Snippets

- Check setting “Save MAPDL db” -> pre-used variables and Named Selections can be used




```
! Plot eines Ergebnisses
! white background:
/RGB,INDEX,100,100,100, 0
/RGB,INDEX, 80, 80, 80,13
/RGB,INDEX, 60, 60, 60,14
/RGB,INDEX, 0, 0, 0,15

resume,file,db      !MAPDL-db einleser
set,last    ! Letzten Datensatz einles
/SHOW,PNG   ! Gibt alle folgenden Plot
!… Bild-Einstellungen machen (Selecti
esel,s,ename,,185,187 ! nur Solids
/TITLE, Element Solution Equivalent S
plesol,s,eqv  ! Element Solution - Un

/SHOW, CLOSE  ! Leert buffer und schl
ALLS
```

Evaluation of Results - Max Tag Adjust to Visible

Å For large assemblies