Small Business Innovation Program (SBIR) Phase II Program – Final Report

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Topic Number 2. Increasing Adoption of HPC Modeling and Simulation in the Advanced Manufacturing and Engineering Industries
Subtopic: Turnkey HPC Solutions for Manufacturing and Engineering

Grant Award No. DE-SC0009494 to Engineering Mechanics Corporation of Columbus

PI: Frederick W. (Bud) Brust

Adoption of High Performance Computational (HPC) Modeling Software for Widespread Use in the Manufacture of Welded Structures

to

Office of Science

US Department of Energy

Washington, DC

by

F. W. Brust, E. Punch, E. Twombly, S. Kalyanam,
J. Kennedy, G. Hattery (Emc^2)

J. Mach, J. Webb, (Caterpillar), R. H. Dodds (Consultant)
J. Nicklas, B. Gohar, D. Hudak, A. Chalker (Ohio Super Computer Center)

Engineering Mechanics Corporation of Columbus
3518 Riverside Drive, Suite 202
Columbus, OH 43221
Phone/Fax (614) 459-3200/6800
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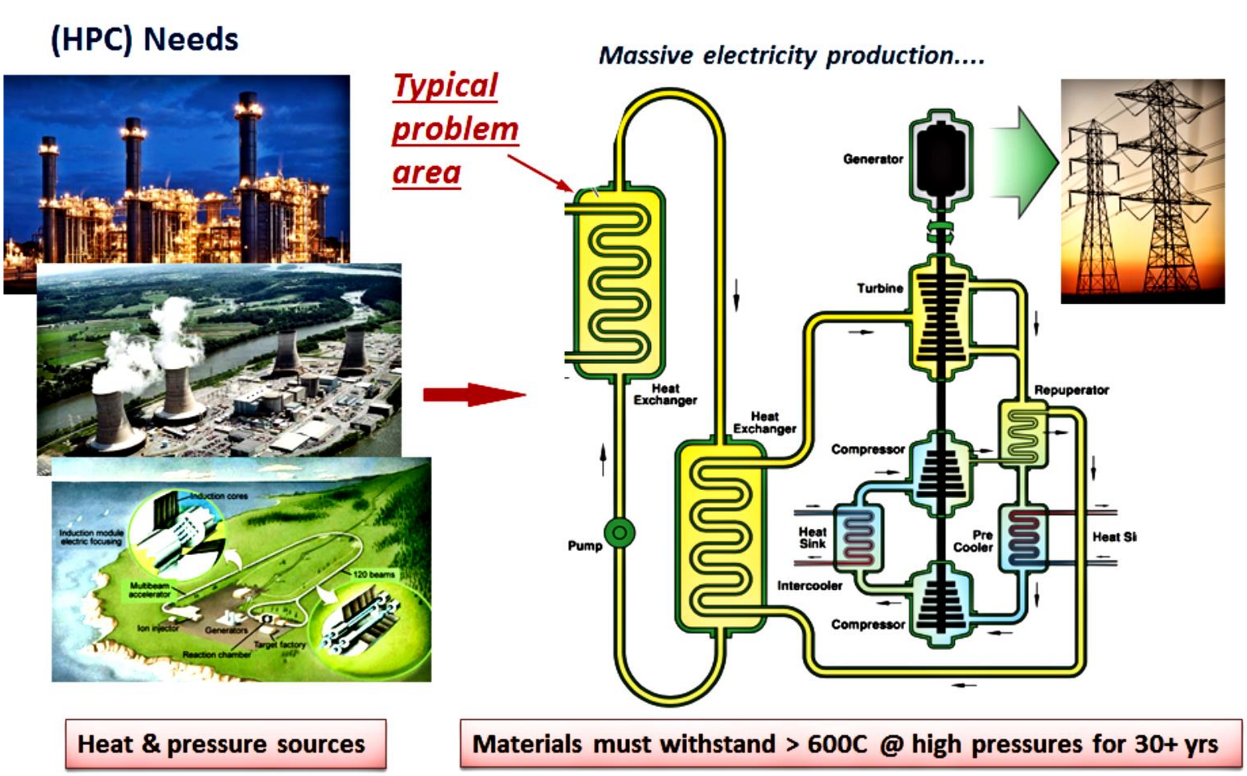
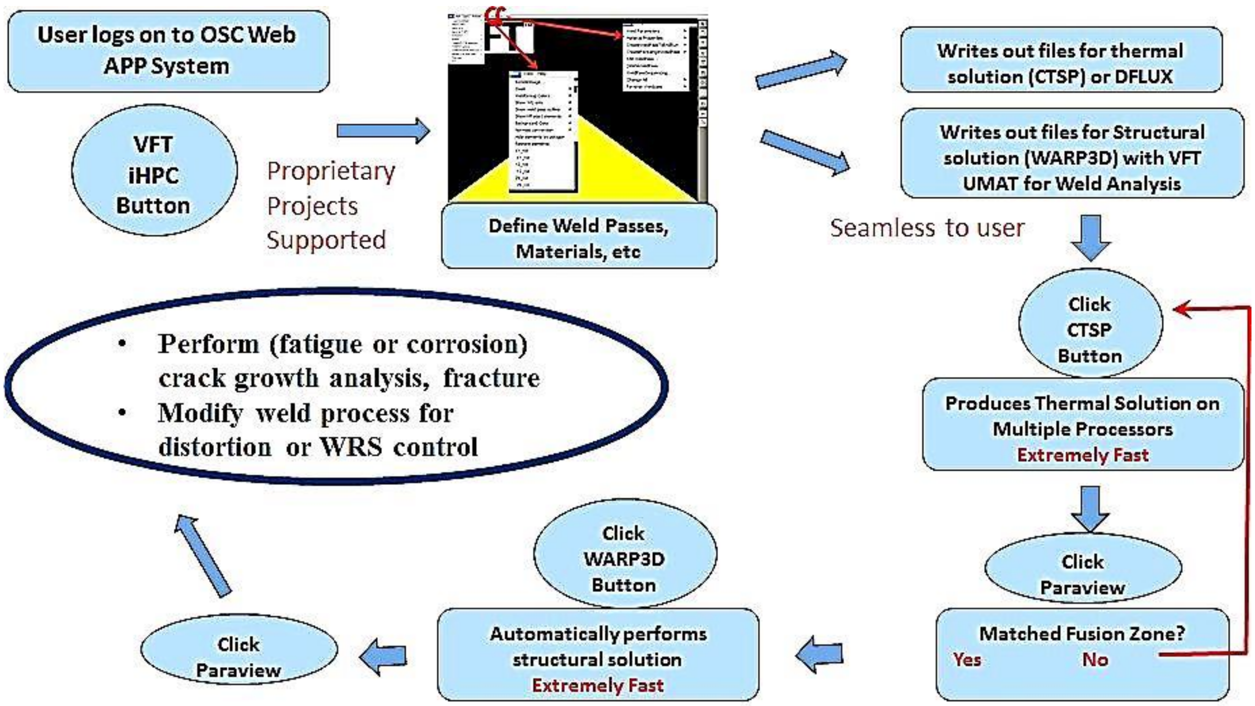
EXECUTIVE SUMMARY

This report summarizes the final product developed for the US DOE Funding Opportunity Number DE-FOA-0000760 Small Business Innovation Research (SBIR) Phase II grant made to Engineering Mechanics Corporation of Columbus (Emc^2) between April 16, 2014 and August 31, 2016. This program was part of Topic 2 - Increasing Adoption of HPC Modeling and Simulation in the Advanced Manufacturing and Engineering Industries; Subtopic: Turnkey HPC Solutions for Manufacturing and Engineering. The program name is 'Adoption of High Performance Computational (HPC) Modeling Software for Widespread Use in the Manufacture of Welded Structures'. ***This report can also be used as VFT documentation and provides a number of tutorials for the new user.***

During the efforts of this SBIR grant, Emc^2's *Virtual Fabrication Technology (*VFT®) weld simulation program was developed to perform efficiently in a high performance computing (HPC) environment on a platform to permit easy and cost effective access to the code for small companies. The need for HPC to address highly nonlinear problems of mathematical physics has emerged as a critical technology in recent years. Some important applications in the energy development are illustrated below. Computational weld modeling for large fabrications can be extremely time consuming requiring long model development times, extensive computational times and resources, and modeling specialists. Moreover, since the final weld process requires iterations in order to achieve the most efficient design, multiple analyses are often required to produce the final optimized product fabrication.



The VFTApp system on the AweSim platform at the Ohio Super Computer Center (OSC) is a 'point and click' process that does not require a weld modeling expert to use. The VFTApp process is illustrated below. The user first obtains an account on OSC and clicks on the VFT iHPC button. The weld model is imported into the graphical user interface (GUI) where weld passes, weld parameters for each pass, material properties, etc. are defined. Next the user automatically writes out all files necessary to perform the thermal and structural portions of the analysis. The user then clicks on the thermal solution button (CTSP below) which automatically performs the weld thermal solution on multiple processors very rapidly. Next the user visualizes the temperatures by clicking on the 'ParaView' button to ensure that the temperatures are correct and the fusion zone is matched. Following this step, the user clicks on the 'WARP3D' button to perform the structural analysis using multiple processors automatically and then clicks on the 'ParaView' button to observe the predicted distortions and weld residual stresses. Finally service performance is gaged. For examples, questions are considered such as: Are distortions within tolerance? Are the weld residual stresses (WRS) at critical locations controlled so that fatigue, corrosion, and fracture issues are managed? WRS can have a strong influence on fatigue and corrosion performance and must be considered. If goals are not met in this iteration, the user repeats the cycle again until the service goals are met.



Emc^2's DOE SBIR Phase II effort successfully adapted Emc^2's *Virtual Fabrication Technology (*VFT®) weld simulation program to perform efficiently in a high performance computing (HPC) environment independent of commercial software on a platform to permit easy and cost effective access to the code. These efforts provide the key for small and medium (SME) sized enterprises to have access to a sophisticated and proven methodology that is quick, accurate and cost effective and available "on-demand" to address weld-simulation, fabrication, and service problems prior to manufacture. In addition, other organizations, such as Government agencies and large companies, may have a need for spot use of such a tool. The open source code, WARP3D, a high performance finite element code mainly used in fracture and damage assessment of structures, was modified so that computational weld problems can be solved efficiently on multiple processors and threads with VFT®. The thermal solver for VFT®, based on a series of closed form solution approximations, was enhanced for solution on multiple processors greatly increasing overall speed. In addition, the graphical user interface (GUI) has been re-written to provide SMEs access to an HPC environment (The Ohio Super Computer Center) to integrate these solutions with WARP3D in a seamless manner. The GUI is used to define all the weld pass descriptions, number of passes, material properties, consumable properties, weld speed, etc. for the structure to be modeled. The GUI was extensively improved to make it extremely user-friendly. Finally, an extensive outreach program to educate and market this capability to fabrication companies was undertaken. This access route will permit SMEs to perform weld modeling to improve their competitiveness at a reasonable cost. All of these improvements are detailed in this final report. Part of this report will also serve as the USER Manual for VFT on the OSC AweSim system.

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1 INTRODUCTION

This report summarizes the final product developed for the US DOE Funding Opportunity Number DE-FOA-0000760 Small Business Innovation Research (SBIR) Phase II grant made to Engineering Mechanics Corporation of Columbus (Emc^2) between April 16, 2014 and August 31, 2016. This program was part of Topic 2 - Increasing Adoption of HPC Modeling and Simulation in the Advanced Manufacturing and Engineering Industries; Subtopic: Turnkey HPC Solutions for Manufacturing and Engineering. The program name is 'Adoption of High Performance Computational (HPC) Modeling Software for Widespread Use in the Manufacture of Welded Structures'. ***This report can also be used as VFT documentation and provides a number of tutorials for the new user.***

Many US companies have moved fabrication and production facilities off shore because of cheaper labor costs. A key aspect in bringing these jobs back to the US is the use of technology to render US-made fabrications more cost-efficient overall with higher quality. One significant advantage that has emerged in the US over the last two decades is the use of virtual design for fabrication of small and large structures in weld fabrication industries. Industries that use virtual design and analysis tools have reduced material part size, developed environmentally-friendly fabrication processes, improved product quality and performance, and reduced manufacturing costs. Indeed, Caterpillar Inc. (CAT), one of the partners in this effort, continues to have a large fabrication presence in the US because of the use of weld fabrication modeling to optimize fabrications by controlling weld residual stresses and distortions and improving fatigue, corrosion, and fracture performance.

This report describes Engineering Mechanics Corporation of Columbus' (Emc^2's) DOE SBIR Phase II final results to extend an existing, state-of-the-art software code, *Virtual Fabrication Technology (*VFT®), currently used to design and model large welded structures prior to fabrication - to a broader range of products with widespread applications for small and medium-sized enterprises (SMEs). VFT® helps control distortion, can minimize and/or control residual stresses, control welding microstructure, and pre-determine welding parameters such as weld-sequencing, pre-bending, thermal-tensioning, etc. VFT® uses material properties, consumable properties, etc. as inputs. Through VFT®, manufacturing companies can avoid costly design changes after fabrication. This leads to the concept of joint design/fabrication where these important disciplines are intimately linked to minimize fabrication costs. Finally service performance (such as fatigue, corrosion, and fracture/damage) can be improved using this product.

Emc^2's DOE SBIR Phase II effort successfully adapted VFT® to perform efficiently in an HPC environment independent of commercial software on a platform to permit easy and cost effective access to the code. This provides the key for SMEs to access this sophisticated and proven methodology that is quick, accurate, cost effective and available "on-demand" to address weld-simulation and fabrication problems prior to manufacture. In addition, other organizations, such as Government agencies and large companies, may have a need for spot use of such a tool. The open source code, WARP3D, a high performance finite element code used in fracture and damage assessment of structures, was significantly modified so computational weld problems can be solved efficiently on multiple processors and threads with VFT®. The thermal solver for VFT®, based on a series of closed form solution approximations, was extensively enhanced for solution on multiple processors greatly increasing overall speed. In addition, the graphical user interface (GUI) was re-written to permit SMEs access to an HPC environment at the Ohio Super Computer Center (OSC) to integrate these solutions with WARP3D. The GUI is used to define all weld pass descriptions, number of passes, material properties, consumable properties, weld speed, etc. for the structure to be modeled. The GUI was enhanced to make it more user-friendly so that non-experts can perform weld modeling. Finally, an extensive outreach program to market this capability to fabrication companies was performed. This access will permit SMEs to perform weld modeling to improve their competitiveness at a reasonable cost. All of these improvements are detailed in this final report and all milestones for completion of the project were completed.

2 BACKGROUND AND PROBLEM DEFINITION

The need to join metallic parts/pieces to achieve final product configuration often employs welding as the joining process. Welding is the preferred joining process for many reasons but to some extent depends on the application. For example, construction of buried pipelines that transport high pressure gases and other energy products typically employs welding of pipe sections because of the inherent leakage problem associated with pipe sections joined by bolted flanges. Also, products that are weight sensitive use welding to join structural parts/pieces because of added weight associated with other joining processes. Indeed, some next generation commercial space flight vehicles are using welded aluminum super structures which require light weight construction[*]. Additionally, welding is the only joining process that can be used in some applications because of geometry or restricted space associated with the product, e.g. stiffeners used in construction of ship panels.

However, welding has some inherent drawbacks and, if not accounted for in early product design, can lead to time consuming, non-value activities that add cost and lengthen time to achieve final product configuration. Distortion and residual stress states are two primary anomalies that can, and often do, occur as a result of welding metal parts/pieces. In particular, distortion due to welding usually requires some sort of re-work such as mechanical pressing, flame straightening, and others (see for instance Reference [4]) to reduce welding effects on final product configuration. Residual stresses induced by welding can, at a minimum, reduce useful life of the structure (corrosion and fatigue) and increase susceptibility to fracture. In the past, and still to a significant degree for the present, effects of distortion due to welding have been addressed by extensive examination of welding processes (torch speed, heat input, consumables, sequencing, fixturing, etc.). These studies result in an expensive and time consuming iterative physical process with no guarantee of achieving final optimal product configuration and performance goals.

Nonetheless, virtual (computational-based) weld modeling/simulation design and analysis tools have been used in the heavy materials industry sector over the past 20 years and the few companies that use these tools have enjoyed significant success in fabrication of products through improved product performance with lower costs to manufacture. Weld modeling tools permit the designer to address distortion and residual stress concerns due to welding prior to fabrication. Also, use of weld modeling tools allows distortion control strategies to be determined in a matter of a few days, not weeks or months as is required when only an iterative, physical approach is employed. Weld modeling and analysis methods can be used very effectively to determine best practices for weld repair and this methodology has been successfully employed for joining (welding) dissimilar metal applications. Members of the industrial sector that have employed virtual design and analysis tools have realized products that have reduced material parts size, more environmentally-friendly fabrication processes, improved product quality and performance, and reduced costs. Indeed, Emc^2 has seen a surge of requests for VFT® from off-shore manufacturers which have been rejected in order to keep this technology's competitive advantages situated in the US.

[*] Emc^2 is currently working with a private company on this proprietary matter.

3 THE VFT® SYSTEM: HIGH LEVEL

3.1 History and Current VFT Development

VFT® is a sophisticated, mathematics/physics-based computer code system that simulates the weld process†. The weld process is a highly non-linear and difficult phenomenon to capture. The weld process involves melting, removal and re-depositing of material, continuous deposition of new weld material, and annealing in the heat affected zone. Prior to Emc^2's DOE SBIR Phase I award, VFT® exclusively employed a commercially available software code as the system solver. As such, the user was required to have a license for this commercial code (pay a fee) to solve the welding problem via VFT®. For large fabrications with many welds, the user must have access to multiple processors and corresponding license access for these additional processors in order to obtain results in a high performance environment. Also, the major method to input data and produce the necessary files to perform the computational weld analysis (weld pass description, number of passes, material properties, consumable properties, etc.) is through a graphical user interface (GUI) tied to the commercial solver.

The VFT® program flow through the OSC AweSim portal is illustrated in Figure 1. The GUI is used to set up the weld problem for the structure of interest. After definition of the weld passes, material inputs, etc., the GUI writes out the thermal code (CTSP) inputs and the WARP3D inputs automatically, solves the thermal problem very rapidly on multiple processors and the corresponding WARP3D structural problem while automatically managing the numerous weld specific data files and results files. This is all through 'point and click' visual access and the user does not need to know details of the analysis process. After solution the visualization program, ParaView, is invoked for results assessment. The user might not achieve the service goals of weld residual stress or distortion from this first analysis. This would require additional iterations using the GUI to modify weld sequence, weld parameters, pre-camber fixtures (or many other weld control features) as discussed later and going through the process again‡. Industrial outreach and marketing the VFT® product along with education and training was important and also performed as part of this program.

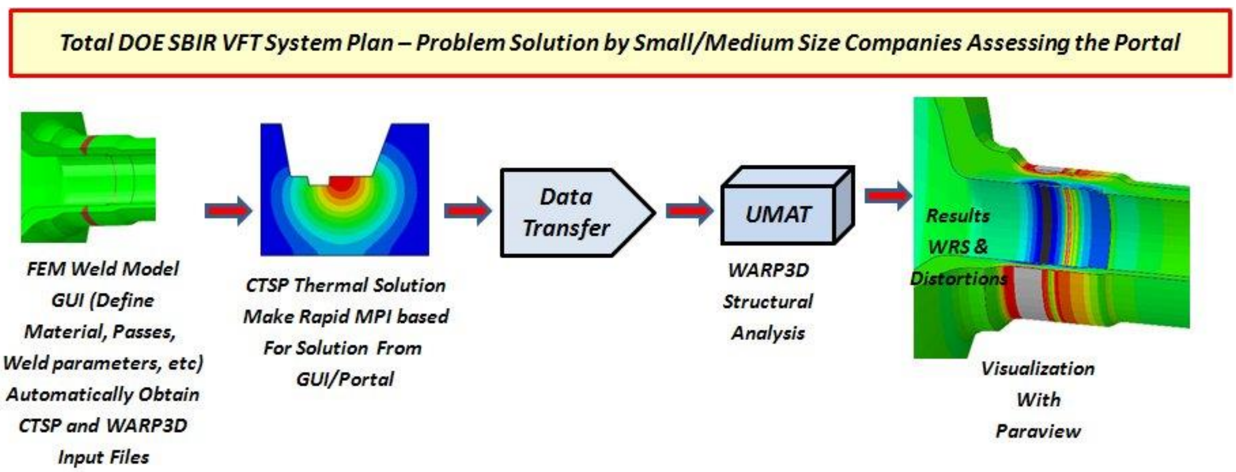


Figure 1 VFT® weld modeling procedure with open source solution process

† Note: Cutting and forming analyses may also be performed via VFT® but only as a subsidiary goal.

‡ Future activities will involve automating a weld optimization procedure but this was outside Phase II budget.

3.2 Overview of the VFT System on the Ohio Super Computer Center

The VFT system resides as a 'point and click' process at the High Performance Computing (HPC) Ohio Super Computer Center (OSC) as part of the 'AweSim' system. In order to request access to VFT on AweSim the following procedure should be followed:

1. Go to ***awesim.org*** and click "Sign Up". In the signup form, to the Additional Information: "How did you find out about this site?" section add this comment: "EMC2: to access VFT". Once we verify and approve your request we will grant you access to VFT and send your user name/password information.
2. Login to ***awesim.org*** with your AweSim OSC HPC account by clicking "Log In" on the ***awesim.org*** site.
3. The dashboard should appear, with a title "EMC2". Click on the VFT link to launch VFT.

After obtaining access to VFT accesses to the system is through a browser with the address for VFT provided from the OSC sign-up. The following screen should appear (Figure 2). The user enters their AweSim assigned user name and password and clicks the 'login' button.

Figure 2 OSC AweSim login site after accessing the system

After login the user is taken to the VFT application (app) shown in Figure 3. AweSim has many other HPC apps available but the user will be directed to the VFT app after signing up. Here the user clicks on the VFT Sim app seen in Figure 3 (the 'click' arrow in this and the following figures is shown with the red arrow). The VFT AweSim app on the OSC System provides high speed access from anywhere in the world.

After clicking on the VFT app the screen in Figure 4 appears. As indicated by the red 'click' arrows in Figure 4 there are several options a VFT user can choose at this point. Clicking Documentation in the upper right will provide information and guides for the user including practice meshes for self-guided learning along with tutorials. Clicking on the 'Open Sessions' button will open prior sessions (and models) that the user has worked on before. The 'Add meshes' button will open a new mesh model for the user to define for VFT analysis. Each of these is described separately below.

Figure 3 VFT weld simulation app

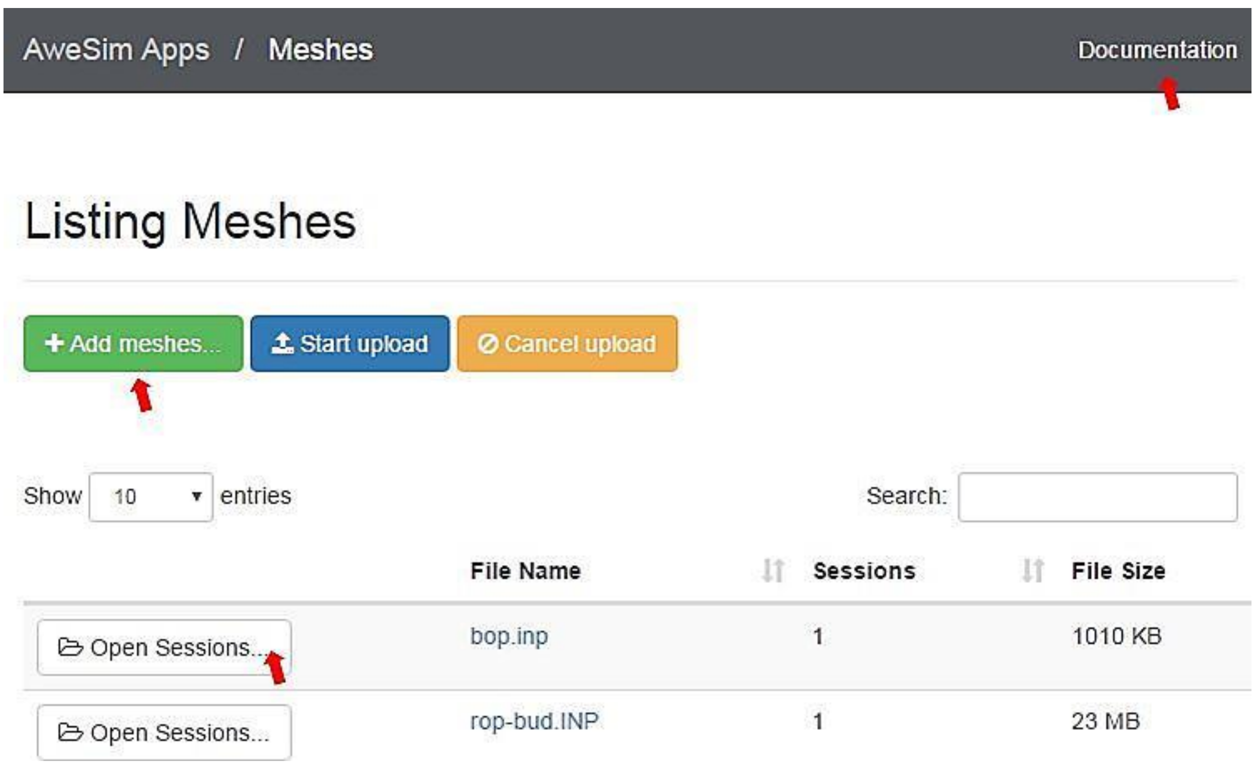


Figure 4 The VFT AweSim app start page

Documentation

Requirements

Required:

- Windows XP, 7, 8, 10
- AweSim Connect v0.90+

Optional:

- VFTSolid v1.3.1 Win32 (Dec. 30, 2016)

AweSim Connect Setup

VFT Workshop (03/15/16 - 03/17/16)

The following powerpoint slides were given during the Spring 2016 VFT workshop hosted at the Ohio Supercomputer Center. You can find the example input meshes in the below Examples section.

Examples

Here you can find a multitude of example meshes. Some examples include constraint files as well as restart files.

Example	Files	Walkthrough
bop	bop.inp	
boss	boss.inp	

Manuals

Here you can find an array of manuals and documentation on the various VFT workflow components.

Figure 5 The VFT AweSim app Documentation page (condensed)

3.2.1 Documentation

Figure 5 shows the (condensed) page that appears for documentation. VFT system requirements are specified. Under 'Optional' requirements the user can download the VFTSolid graphical user interface (GUI) to their desktop if they choose. This might be useful for the user as they learn the VFT system without having to be connected to the super computer. The GUI will run on Windows. The user can define the weld problem of interest and then save it as a 'VFTr' file. This file can then be uploaded to the OSC AweSim site and opened there to perform an analysis. Referring to Figure 5, the AweSim connect setup information is provided next. The user should not have to worry about this as OSC will help in setting up VFT for the user the first time.

The final report is also available for download. This can be used as a manual and with the tutorials. In addition, the tutorials can be downloaded separately with the example input files for the user to learn the system.

Additionally, documentation on a VFT workshop that occurred in the Spring of 2016 for users is included in this part of the App site. A number of PowerPoint tutorial files are provided for download that can help the user learn VFT. These include slides for Workshop Agenda, VFT summary and app use, summary slides for OSC, example tutorials, solutions, and tutorial files to use for practice. The user is encouraged to download these files, study them, and run examples prior to solving their own problems.

Next are example files the user can download and practice solving along with tutorials. There are a number of these examples with only two of them shown in Figure 5. Finally manuals and other VFT related reports and publications are available for all VFT system components. These can be useful for doing 'advanced' modeling work.

3.2.2 Open Sessions

As seen near the bottom in Figure 4 the user can open sessions that have been worked on before. All prior sessions are saved on the system for the user until they delete them. The user can open prior sessions to view results, modify the analysis (change weld sequences, heat input, materials, etc.) There can be many separate analyses associated with a mesh that was used for a particular session. Each separate analysis associated with a session will be shown and the user can also define another analysis within this same session.

3.2.3 Add Meshes

Finally, as shown in the upper left of Figure 4 the user can start a new set of sessions with a new mesh clicking on 'Add meshes'. This will permit the user to upload a new VFT weld mesh from their computer to begin another analysis. This process is described in Section 3.3 next.

3.3 High Level Procedure for Performing a New VFT Analysis

When the user clicks 'Add meshes' (Figure 4 upper left) the following sequence occurs. The user's desktop file folder appears. The user navigates to the mesh to be used for the VFT weld analysis.[§] For this example we chose to get a simple mesh called 'Simple_Tee.inp' (see sequence in Figure 6) and the user clicks the 'Upload' button. The mesh is uploaded to AweSim, the user clicks 'Add session' in Step 3. The user then launches the session (Step 4) and the GUI opens with the mesh.

[§] To use VFT a mesh must already have been developed. The type of mesh necessary for VFT analysis is described later.

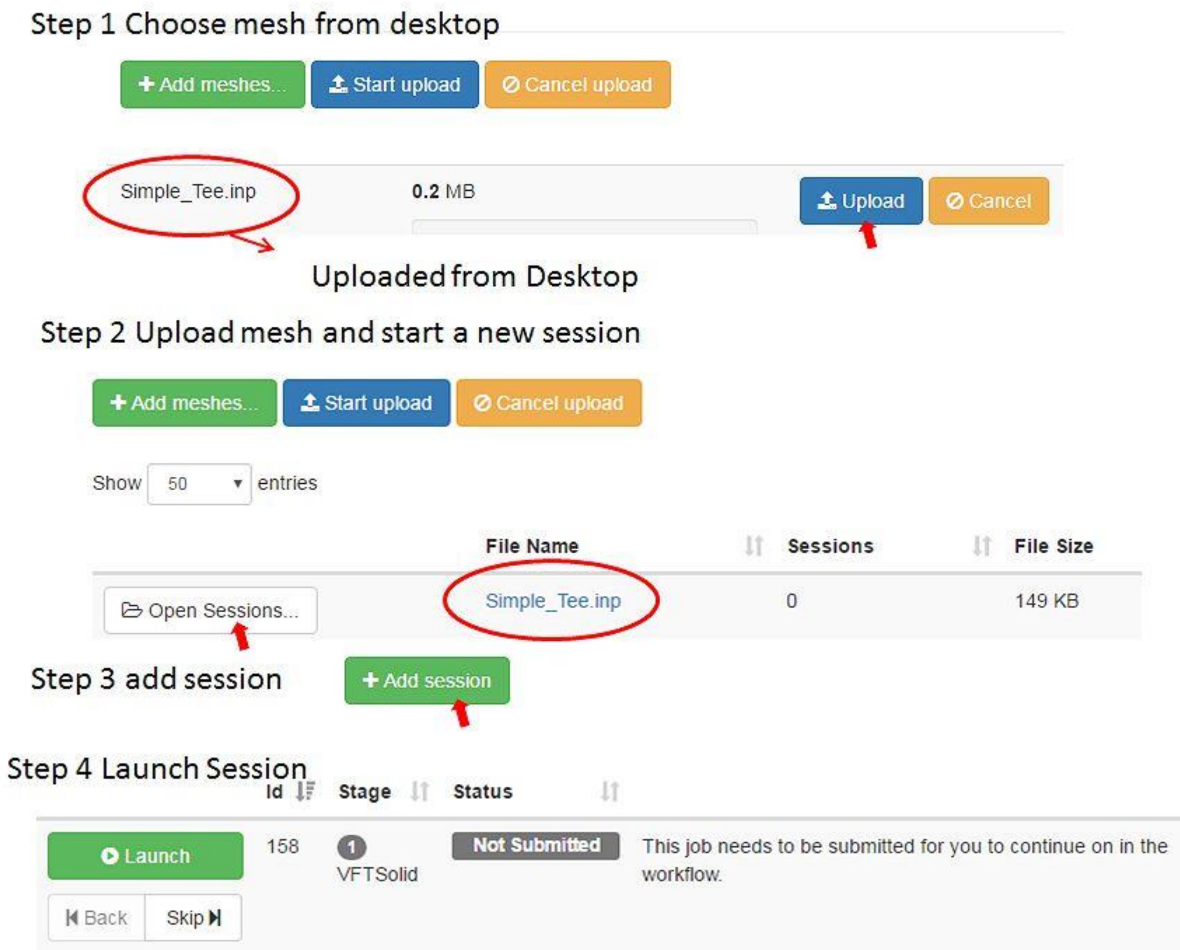


Figure 6 Choosing mesh, upload, and launch VFTSolid

After the user opens the session (Step 3 Figure 6) the full screen for running VFT opens as shown in Figure 7. In Figure 7 the screen shows an ID number (which is the number on the OSC system associated with the directory the analysis is performed in – not necessary for the user to know this). There are four (4) stages involved in the total analysis. Stage 1 is the VFTSolid GUI (shown in Figure 7); Stage 2 is the thermal solution; Stage 3 is the structural solution (using WARP3D); and Stage 4 is visualization of the weld temperatures or final results (weld residual stress or distortions). Under the 'Launch' button are 'Back' and 'Skip' buttons. These are used to go back a stage in the analysis or skip a process and will be described later. On the right bottom of Figure 7 is the 'Thermal' button. This is used to view the weld fusion zone after Stage 2 (thermal solution) is complete. The 'Structural' button is clicked after Stage 3 is complete to view weld residual stresses and distortions.

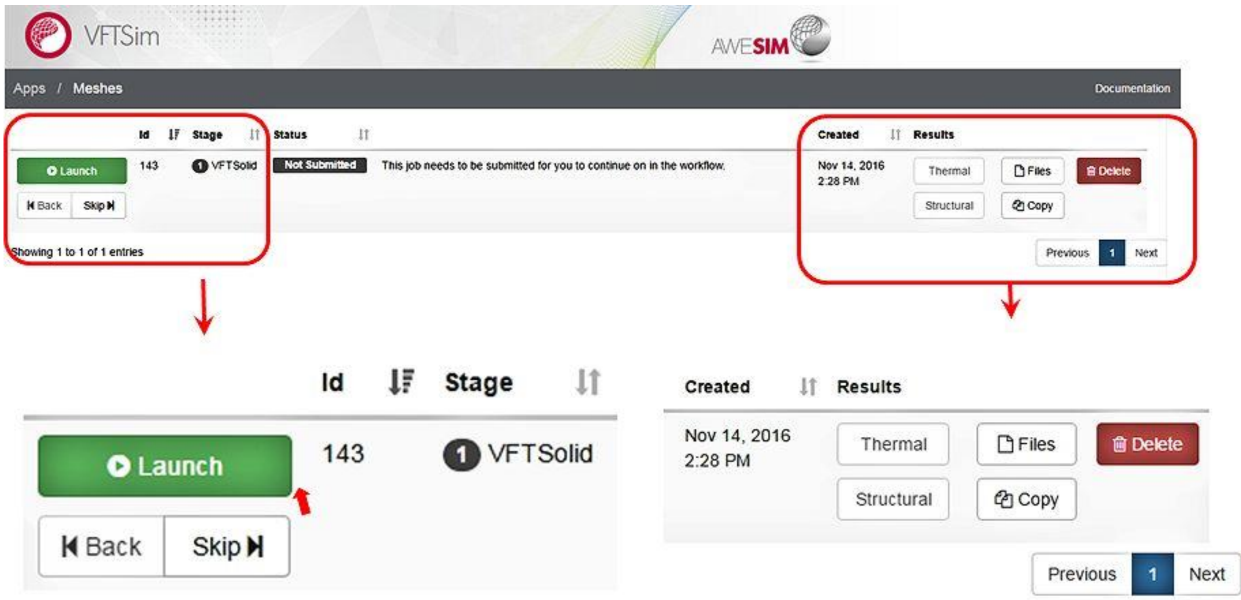
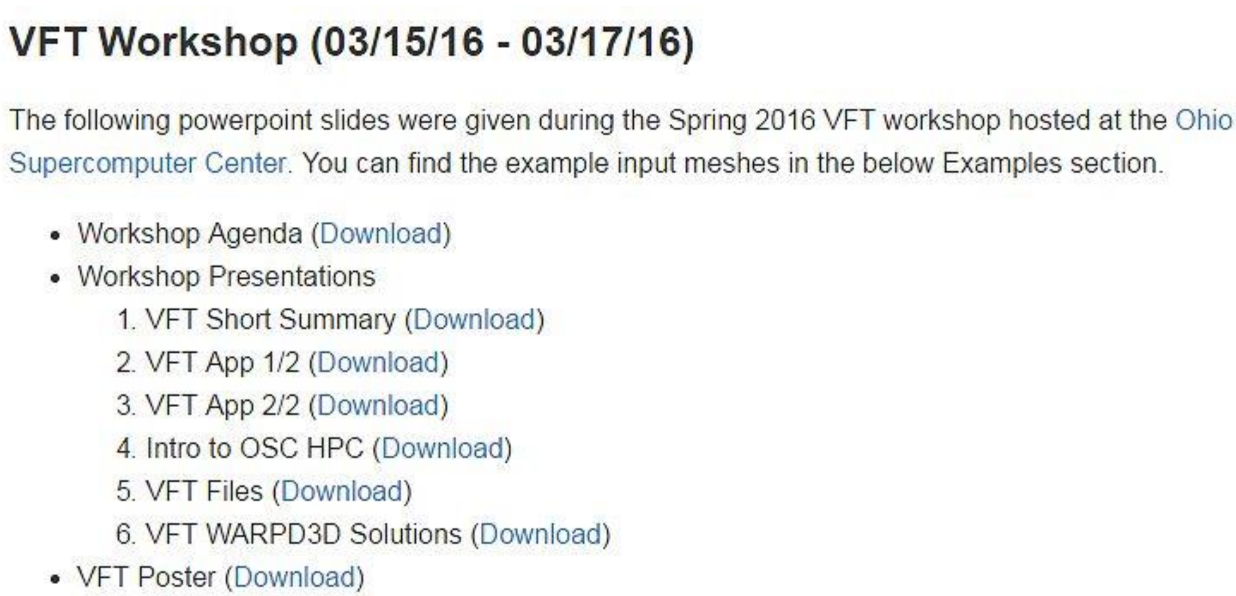


Figure 7 VFTSim screen after opening session



VFT Workshop (03/15/16 - 03/17/16)

The following powerpoint slides were given during the Spring 2016 VFT workshop hosted at the Ohio Supercomputer Center. You can find the example input meshes in the below Examples section.

- Workshop Agenda (Download)
- Workshop Presentations
    1. VFT Short Summary (Download)
    2. VFT App 1/2 (Download)
    3. VFT App 2/2 (Download)
    4. Intro to OSC HPC (Download)
    5. VFT Files (Download)
    6. VFT WARPD3D Solutions (Download)
- VFT Poster (Download)

Figure 8 VFT Workshop training material available for download from Documentation

The 'Files' button is clicked in order for the user to be able to advance to the appropriate directory where the analysis is being performed. This is useful for the advanced user if they wish to make direct changes to any of the files used for the thermal or structural solution prior to solution or to redo the solution with other parameters. The user can also download VFT ParaView results files to their desktop and use ParaView on their desktop to make reports, etc. This is described in the VFT Workshop training slides which are available for download and study as described in Figure 5. Details of the Workshop training and tutorial download material are shown in Figure 8. The file system descriptions can be examined in '5 VFT Files (Download)' seen in Figure 8 and documentation section of the app. Descriptions of all files used are provided in this document. For the average user, knowledge of these files is not important as the VFTApp automatically creates all files necessary for VFT analysis.

Figure 9 illustrates the progression through the stages. When the user clicks ‘Launch’ in the top left screen the VFTSolid GUI, shown in the upper right in Figure 9 for an automotive under body frame, appears. The user then defines materials (for both thermal and structural solutions), all weld parameters and passes, constraints, etc., and then the system automatically writes out all files necessary to perform the thermal and structural solutions. A ‘List of materials’ dropdown box also appears so the user can choose from a library of materials if desired. After the weld problem is defined, the user writes out the thermal and structural files and exits the VFTSolid GUI. It is useful to save the file as a ‘VFTr’ file here so that the user can open the file and make changes in the future if desired. Then back in the VFTApp the user clicks the red ‘Stop’ button.

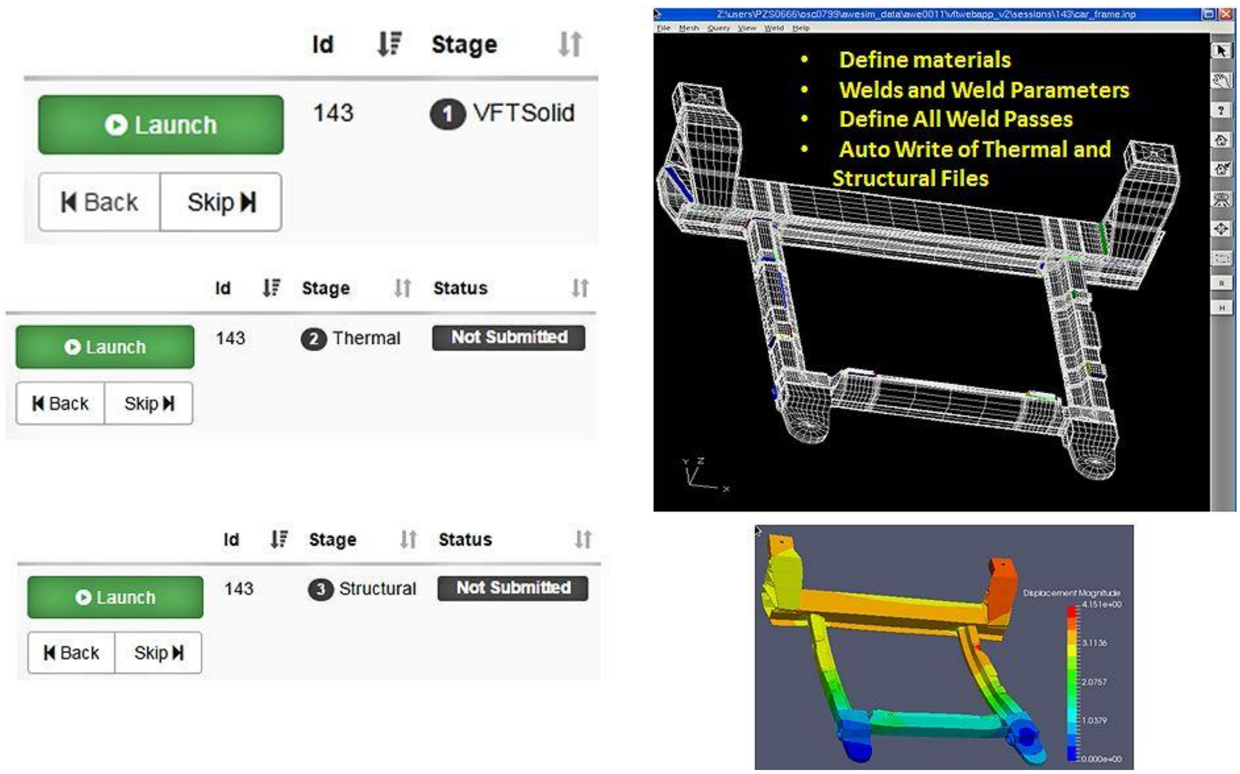


Figure 9 VFT Solution procedure for Stage 1 (launch of VFTSolid GUI), Stage 2 (Thermal Solution), and Stage 3 (Structural Solution using WARP3D). The result is shown in the lower right and represents Stage 4.

The second stage (Stage 2) appears as depicted in the middle left part of Figure 9. The user then clicks on the green ‘Launch’ button and the thermal solution is performed automatically. The user chooses the number of processors to use for the thermal solution when writing out the thermal files in VFTSolid GUI. The thermal solution is very fast and often the user chooses the number of processors that corresponds to the number of welds. So if a structure has 40 welds the user would choose 40 processors for the thermal solution. After the thermal solution is complete the user has the option to view the results to ensure that the fusion zone has been matched.

Additionally, after the thermal solution is complete the system moves to Stage 3 (bottom in Figure 9). The user then launches the structural solution by clicking on the green ‘Launch’ button. A progress bar appears which gages the solution. The solution currently uses 20 processors for the structural WARP3D solution. WARP3D runs very efficiently on multiple processors on the same core and is faster than ABAQUS for instance for similar analyses.

Finally, as seen in Figure 10, Stage 4 represents the completion of the solution. On the middle illustration in Figure 10 Stage 4 automatically appears. The user can go back to different stages of the solution by clicking the ‘back’ button. For instance, if the user clicks back once we go to Stage 3 and can redo the structural solution for instance. Clicking ‘Back’ twice brings us back to the thermal solution. Changes can be made and the solution re-run.

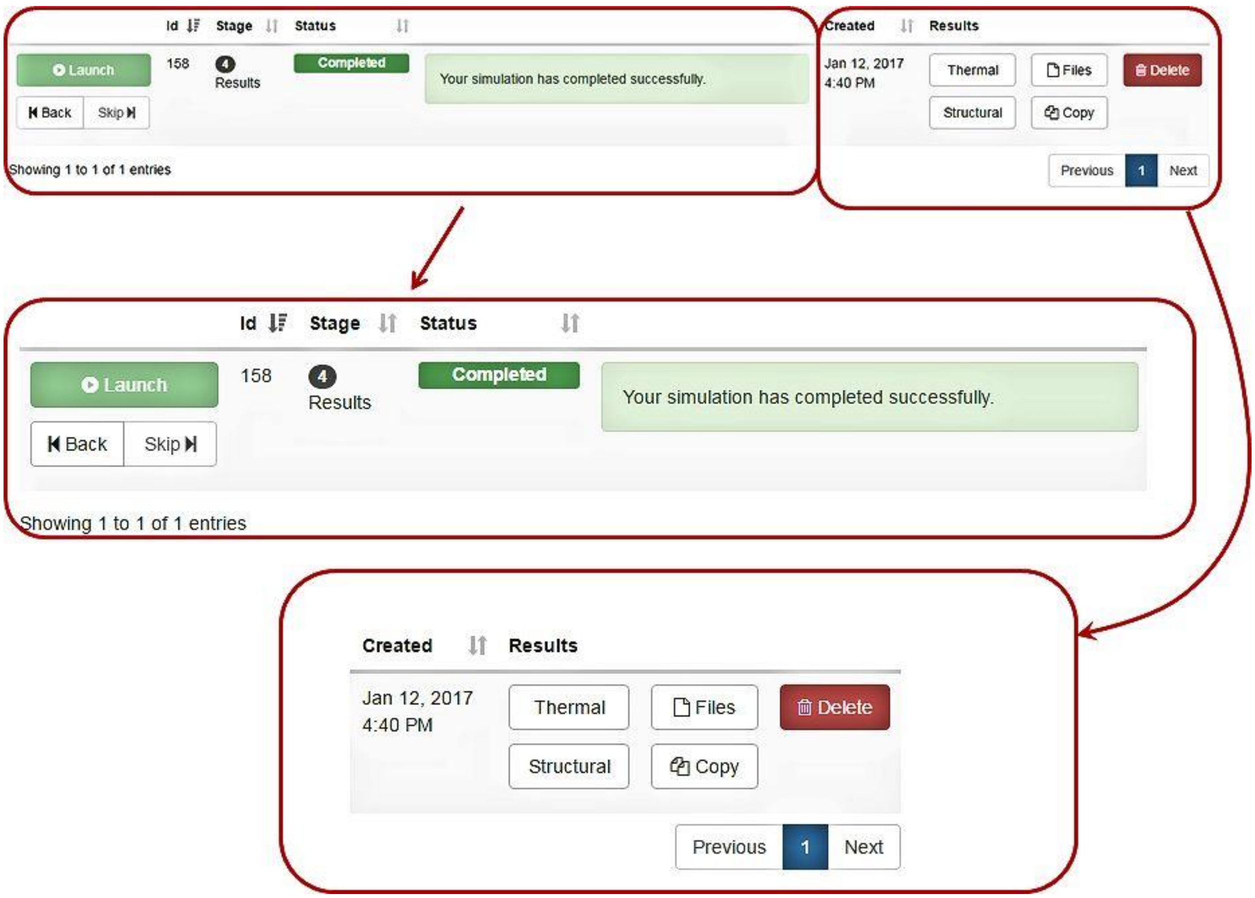


Figure 10 VFT Solution procedure for Stage 4 after solution is complete

At the bottom of Figure 10 the user sees the ‘Thermal’ and ‘Structural’ buttons. These are used to launch the VFTApp solution visualizer. This visualization uses the powerful ParaView code. Note that the ‘Thermal’ button can be used after Stage 2 is complete, before launching the structural solution, to ensure that the weld fusion zone is properly matched. The ‘Files’ button was described above and the ‘Copy’ button can be used to copy results from this analysis to a separate session and then redo the analysis using different inputs, etc. Often the 'Skip' button is used after 'Copy'.

3.4 Autonomous VFT Self Training

Figure 8 describes training slides and materials that can be used by a new user to learn the VFT system. It would be useful for the new user to take a training course. However, even without this the user can learn using these tutorial slides. The definition of weld passes using the VFTSolid GUI can be learned using Slide sets 2 and 3 from Figure 8 (please download from the Documentation section of the VFTApp). A description of the improvements made to VFT by enhancing WARP3D can be found in Slide set 6. Additional material is provided in the following sections where we go through several training tutorials which we recommend the new user work through.

4 THE VFT SYSTEM: DETAILED ANALYSIS TUTORIAL

The following section describes the VFT system in detail. There are four modules:

1. The Graphical User Interface (GUI)
2. The Thermal Solver or Computational Thermal Solution Procedure (CTSP)
3. The Structural Solver using Enhanced WARP3D Open Source Code
4. Visualization of Results using ParaView

In addition, the user may want to perform a 'Restart' analysis (in case divergence occurs for a problem, to add service loads after solution, for repair weld analysis, etc.). These are also discussed.

The general analysis procedure involves the nine steps listed below. As described in earlier sections, VFT computational weld analyses can now be performed using WARP3D. The packages for the WARP3D code have a number of manuals associated with them. The user should become familiar with these manuals prior to using this tutorial. However, the following procedure with the use of the GUI should permit the VFT user to use WARP3D to solve weld problems with minimal need for the WARP3D manuals.

The procedure for a VFT based computational weld analysis is summarized in the nine steps below.

- Step 1. Read the weld based finite element mesh into the GUI (see Figure 9 top illustration). Finite element mesh requirements require that all elements within the welds be extruded 8 node elements. In fact we recommend that all (or most elements) be 8-node bricks for best accuracy. Example meshes are shown during example discussion.
- Step 2. Define the material definition sets and weld parameter sets. Up to 10 materials can be used and as many weld set parameters as desired, although there are usually only a few of these required. Moreover, each weld parameter can be redefined during pass definition.
- Step 3. Define all of the weld passes. This includes the cooling times desired for each pass.
- Step 4. Define boundary conditions. Boundary conditions can also be introduced separately on the users' desktop and uploaded to OSC.
- Step 5. Write out the input file for the thermal analysis (CTSP) along with the number of cores desired for CTSP solution. Usually the user chooses the number of cores to equal the number of weld passes for fastest solution. Also write out input files for the structural solution (WARP3D). The preferred nonlinear solution parameters for weld analysis, and all other parameters needed for the WARP3D analysis are automatically set. The user chooses

the number of ‘Output plot’ files and ‘Restart’ files desired. This also writes out utility routines such as VED needed for the analysis to account for material not yet deposited ahead of the weld torch. While it is useful for the user to be familiar with WARP3D and the corresponding User manuals this is not necessary as the complete input file necessary for analysis is written.

Step 6. Perform CTSP analysis, merge results, and write the files in the format required for WARP3D analysis. This is all done automatically with the GUI. This is done by clicking the ‘Launch Thermal” button (see Figure 9 middle illustration).

Step 7. Perform the WARP3D analysis by clicking on the ‘Launch Structural’ button (see Figure 9 bottom illustration).

Step 8. Examine results in ParaView.

Step 9. If distortion goals or weld residual stress goals are not met, use the GUI to modify pass sequence, boundary conditions, pre-camber definition, etc. and go to Step 5 and repeat to achieve the desired goals.

4.1 Training Materials

As discussed above Figure 8 lists training material that can be downloaded from the VFT AweSim site for the new user to learn the system. We recommend that the new user download these files to their desktop and study them prior to running tutorials. We also recommend that the user download the GUI to their desktop (see Figure 5) to practice using the GUI. Note that the advanced user can define the problem on their desktop and port the files over to OSC if they choose to do so. However, most users will want to use the GUI on the super computer since all analysis is ‘point and click’ on the system.

The workshop material consists of the following.

1. ***VFT Short Summary*** – This provides a summary of the VFT system, historical perspective, overview of the VFT modules, validation examples, and some reference material. Additional material can be obtained from Dr. F. W. Brust at user request (bbrust@emc-sq.com).
2. VFT App 1/2 - Details about the GUI usage and examples are provided.
3. VFT 2/2 - These are similar to VFT App 1/2 and are the latest version. Details about the GUI usage and examples are provided.
4. Introduction to OSC HPC – Overview of the OSC supercomputer system.
5. VFT Files – Discussion of the VFT File system. This is useful for the advanced user.
6. VFT WARP3D Solutions – Details about VFT using WARP3D along with enhancements needed for weld modeling are presented.

4.2 VFT Manuals

VFT manuals can be downloaded (see Figure 5 bottom). The list of manuals for download is listed in Figure 11.

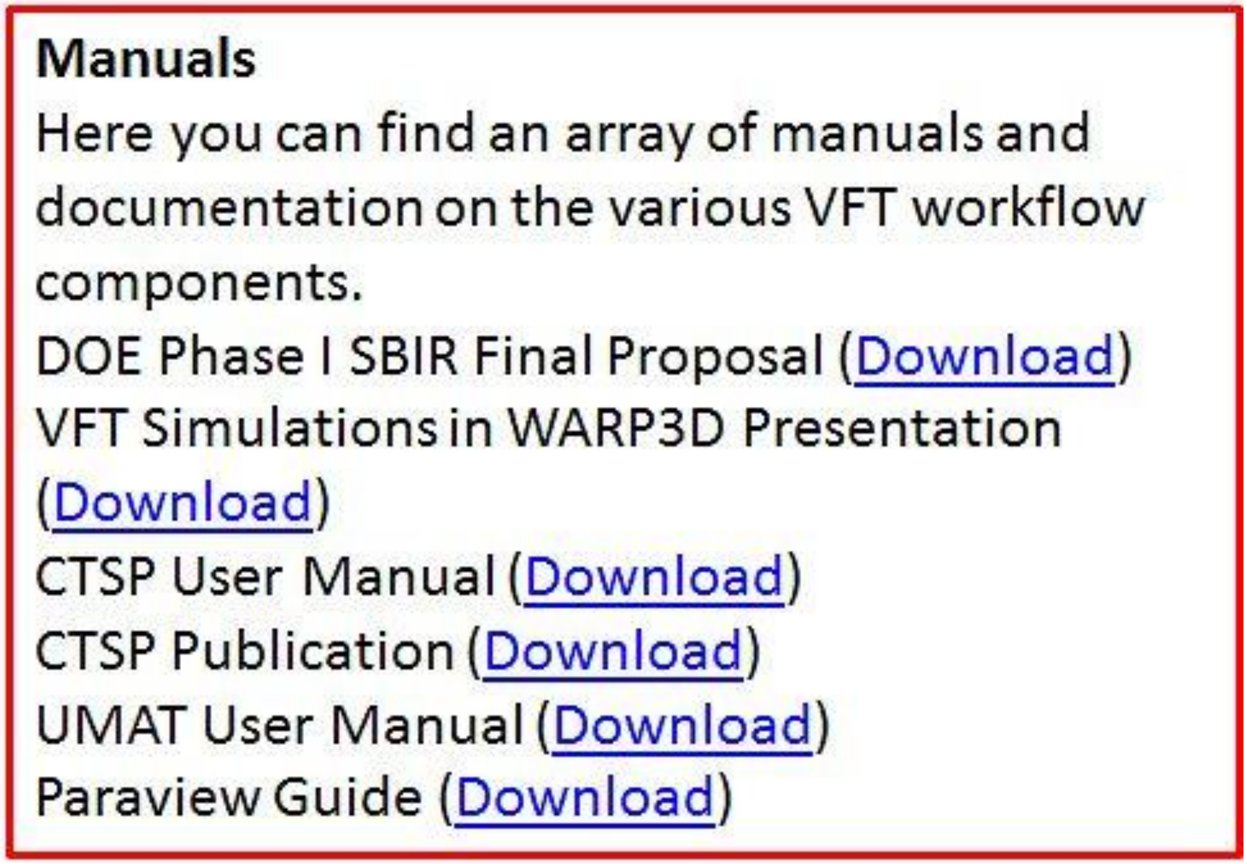


Figure 11 VFT manuals available for download

4.3 Lap Joint Weld Problem

The mesh for the lap weld (lap.inp from Figure 5) should be downloaded to the user's desktop in order to begin this tutorial. The 9 step procedure summarized above will be followed.

Step 1. Click 'Add Mesh' (Figure 4) and upload the 'lap.inp' file from the desktop (Figure 6). Upload mesh, start a new session, and 'Launch' the GUI. The GUI will appear on the screen. As seen in Figure 12 the user opens the 'lap.inp' file and the mesh is available as seen in Figure 13. Note that this is a simple one pass lap weld example. The user must develop a mesh with VFT at present.[**] The *.inp file is read in as an ASCII file which lists nodes, elements, and weld groups only. Extraneous information in these files (for instance additional ABAQUS input file commands) is ignored. The new user is encouraged to download some or all of the input files listed in the Examples section of the VFT Documentation (Figure 5) and open in an 'Editor' to view the format of VFTGUI input files. The general form of these files (for the lap.inp for instance) is shown in Figure 14.

[**] We are working on adding a mesh procedure (automatic) within the GUI but this is not available at present.

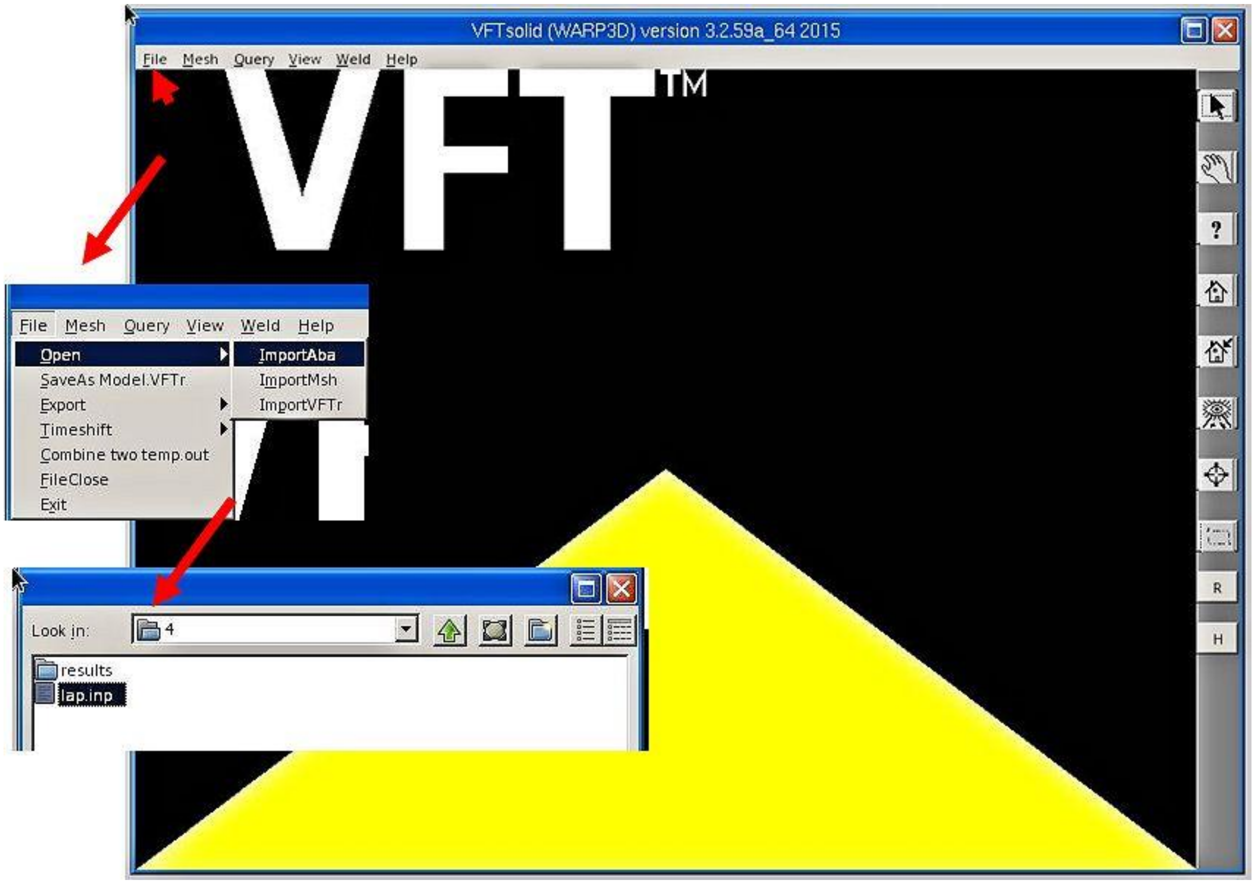


Figure 12 Opening the 'lap.inp' mesh into the GUI

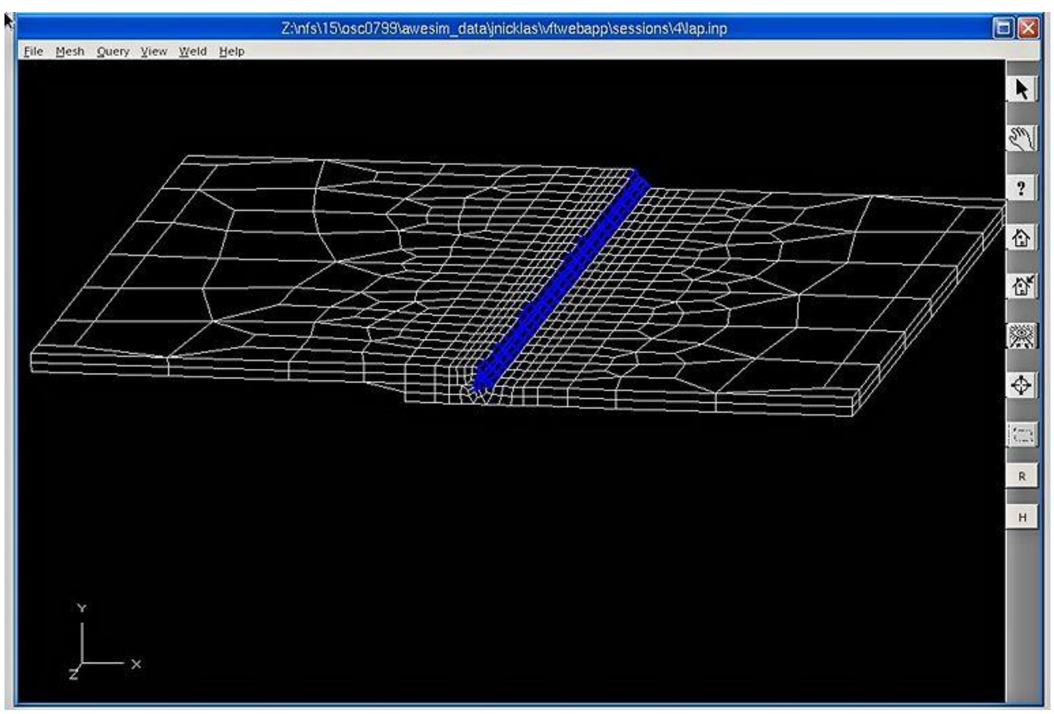


Figure 13 Visualization of the 'lap.inp' mesh in the GUI

As seen in Figure 14 the format is similar to an ABAQUS input file. A '**' can be used to insert comments. Nodes are input using '*NODE' command followed by node number and X, Y, Z coordinates. Elements must be 8-node solid (WARP3D requirement) and are introduced with '*ELEMENT' with element number in Column 1 followed by the 8 node numbers (or less for wedge and tetrahedral elements using WARP3D element input format (ABAQUS also)). Finally, each weld pass group is introduced with '*ELSET,ELSET=wg#' in ABAQUS type format. The name of welds must start with 'w' or 'weld' so that the GUI knows that this group is a weld. The user can list all elements in the group or generate between elements as seen in Figure 14 (for instance 941, 945, 1 represents elements 941, 942, 943, 944, 945. Note that other groups can be defined for instance *ELSET, ELSET=PLATE for other groups that are not part of a weld. This is useful for problems with multiple materials where the plate material is different from the weld material.

```
** COMMENTS
** COMMENTS
*NODE
    1,  -14.00002,    -1.E-7,      0.
    2,  -10.07407,     12.7,       0.
    3, -30.437035,    -1.E-7,      0.
    4, -30.437035,     12.7,       0.
    ......
    ....
*ELEMENT
   1,   50,   51,   76,   75,  124,  126,  176,  174
   2,  124,  126,  176,  174,  125,  127,  177,  175
   3,   51,   52,   77,   76,  126,  128,  178,  176
    ......
    ....
** WP1 ELSET
*ELSET, ELSET=wg1, GENERATE
941,945,1
1188,1190,1
1215,1374,1
*END
```

Figure 14 Input file format for VFT GUI *.inp file (lap.inp here)

Step 2. *Define Materials*. As seen in Figure 15, the user first defines weld input parameters (Amps, Volts, Arc Efficiency, and weld torch speed). Many weld parameter sets can be defined. The arc efficiency may need to be tweaked in order to match the weld fusion zone (discussed later). As a rule of thumb, MIG weld has efficiency of 0.75 and TIG 0.45.[††] Please see the CTSP Manual Figure 11 for more details of units, efficiencies, and the thermal model.

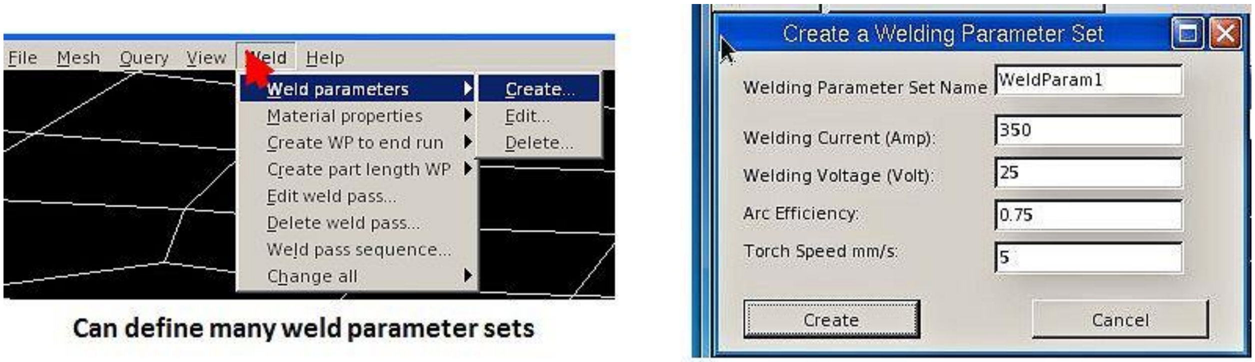


Figure 15 Weld power input parameter definition

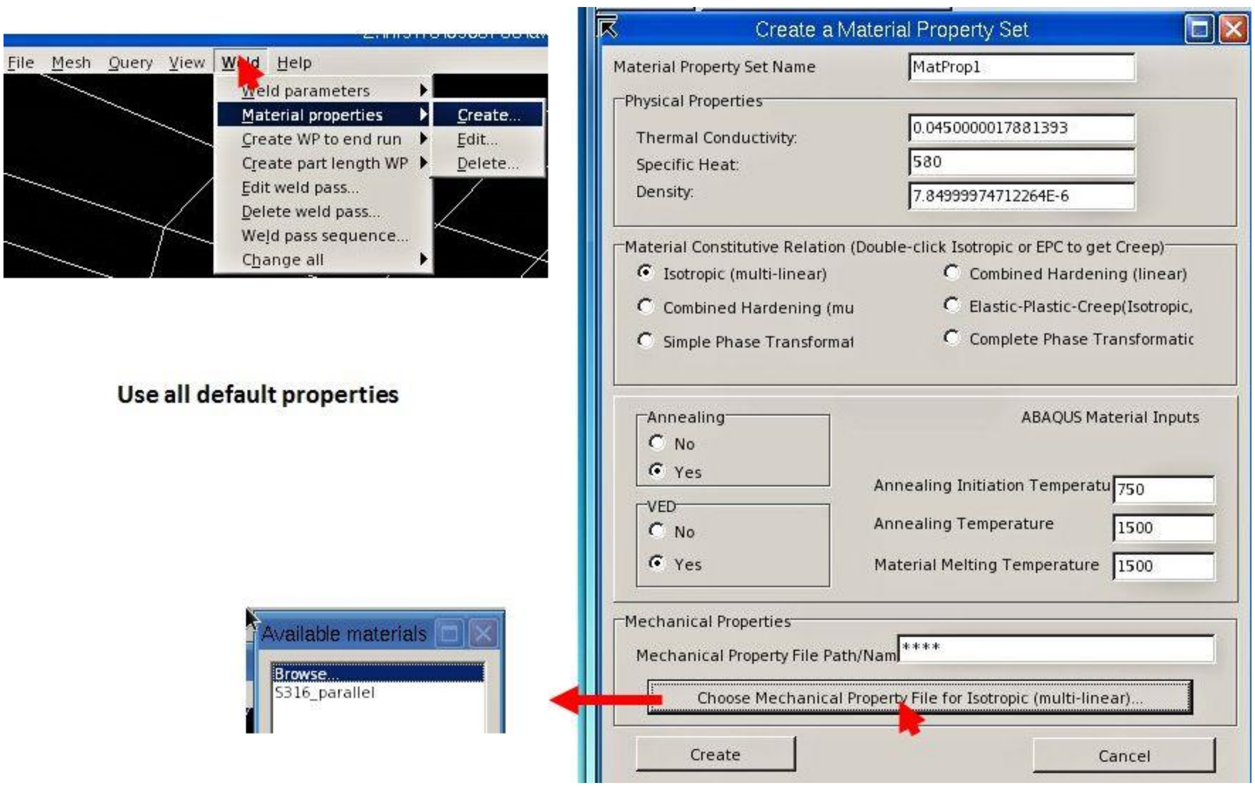


Figure 16 Weld material parameter definition

Figure 16 shows how to define the material properties for a given material (up to 10 materials). The upper box is used to define thermal properties. We have found that using thermal properties

[††] These efficiency numbers for MIG, TIG, and other weld processes (for instance laser or electron beam) may need to be studied for the problem being solved by the user.

at about 300 C produce good results since these properties are weakly dependent on temperature and do not have a large effect on weld temperatures based on extensive validation studies. When the file is opened default parameters for mild steel are placed in the boxes (metric units). Next the user clicks the material constitutive relation to use. The user can choose isotropic hardening, linear or multi-linear (Chaboche) hardening, Elastic-Plastic-Creep (for post weld heat treat modeling), and simple and complex phase transformation plasticity models (based on the Leblond model). The file format for these material constitutive laws is described in the VFT UMAT Manual (Figure 11).

Next the user chooses 'Annealing' and 'VED' and the annealing temperatures. It is recommended that the user always choose 'yes' for both of these parameters. These account for material re-melting and removing of history as weld torches melt virgin or previous weld material and for material that has not yet been deposited (VED). These are defined in the VFT UMAT Manual (Figure 11). For most steels the default values which appear in Figure 16 work acceptably. For aluminum, nickel-based alloys, and some other materials, modification of these parameters results in better performance. See the VFT UMAT for details.

Finally, at the bottom of Figure 16 the user chooses the structural material input file (for WARP3D) to use. When the user clicks 'Choose Mechanical Property File' a library of materials appropriate for the different constitutive laws appears which the user can choose. Alternatively, the modeler can choose a user defined material property file by clicking 'browse'. The user's own material file must be transferred from their desktop to the directory where this analysis is being performed. This is done by clicking on the 'Files' menu (Figure 7). This will direct the user to their desktop where they can drag the file to the correct directory on the super computer where this analysis is being conducted.

Step 3. *Define weld passes.* After defining all weld parameter sets needed and all material properties necessary, the user next navigates to the 'Weld-Create WP' menus. Here we will define this using 'Full' section (other options are discussed later). Referring to Figure 17, after choosing the type of weld pass (here we have 'Create weld pass (WP) to end run – Full Section') the menu box to the right appears. The weld pass and pass sequence number appear at the top and are automatically updated for the user as additional passes are deposited. Next the Joint Type is chosen. The Joint Type options are T-fillet, V-Groove, Lap Joint, and Box-type (see CTSP Manual) and here 'Lap Joint' is chosen. Next Joint shape is chosen from Non-Circular (or general), Full Circle, Part Circle, Girth (Full Circle) or Girth (Partial Circle). The user chooses the type of weld appropriate for the problem (non-circular here). For most problems, even for girth or curved welds the 'non-circular' option will perform satisfactorily.

Next, the user chooses time step control. Default times of 450 seconds for inter-pass cooling time and 5 seconds[‡‡] for inter pass cooling steps appear. The 'Max' and 'Min' Heating times should only be used by an advanced user (see CTSP Manual for these parameters). The user will want to choose a longer time for the final cool down step to ensure that the structure cools to ambient temperatures after all welds are complete. Usually 5000 or 10000 seconds suffices for this depending on the problem. Next the plate thickness on each side of the weld is defined for 'Plate 1' and 'Plate 2'. Figure 17 shows the values chosen for the lap problem. For this case the plates on each side of the lap joint are 12.7 mm thick. Note that the 'Query' button (Figure 16) can be used to find thicknesses and other query items.

[‡‡] VFT time units should be seconds. However, if all units are consistent any units can be used.

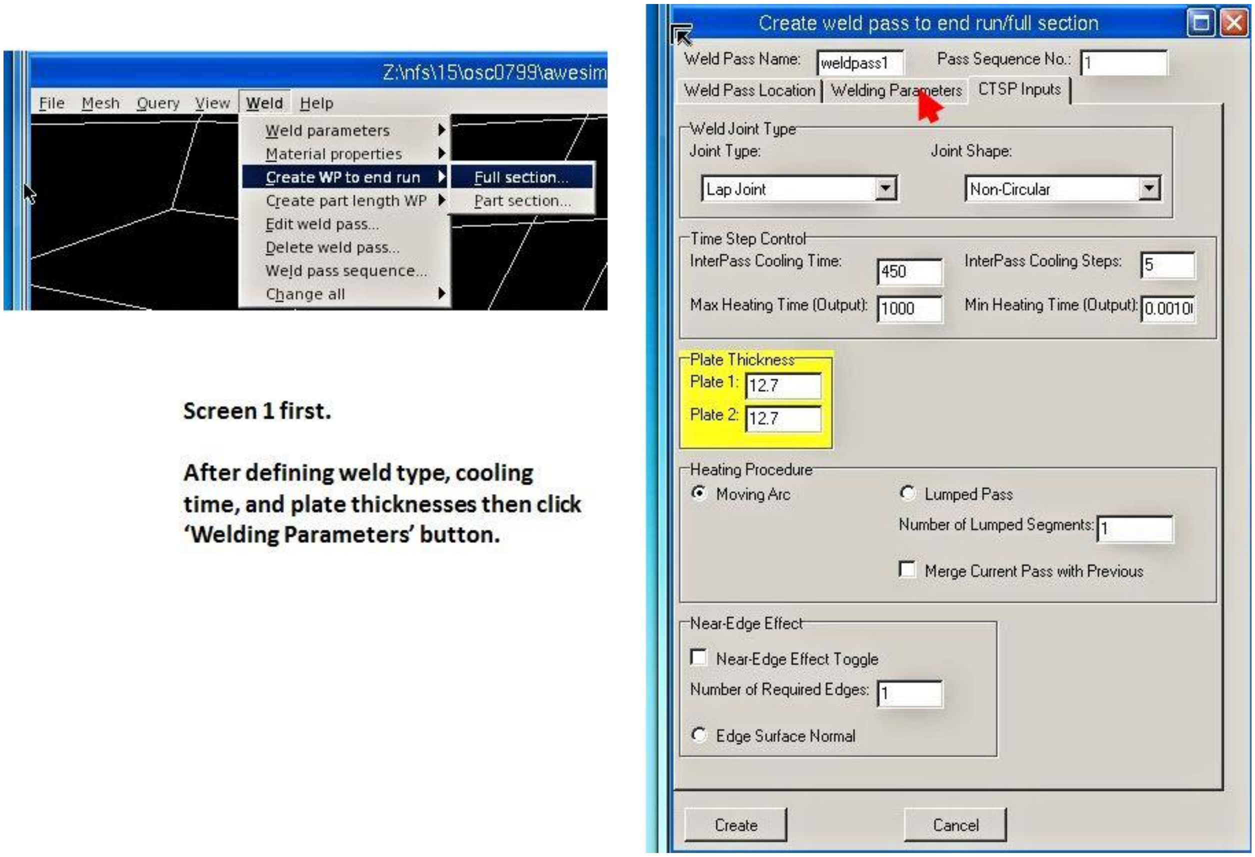


Figure 17 Weld pass definition

After completing this screen the user clicks 'Weld Parameters' tab (Figure 17). As seen in Figure 18 the user then chooses the weld parameter definition set for this pass. The weld parameters and temperature control parameters then populate the box. Note do not change these values. Rather use the values defined for the parameter set.

Screen 2 weld parameters.

Choose Weld Parameter set that you previously defined.

The parameters will populate the dialogue box.

Then click 'Weld Pass Location' button.

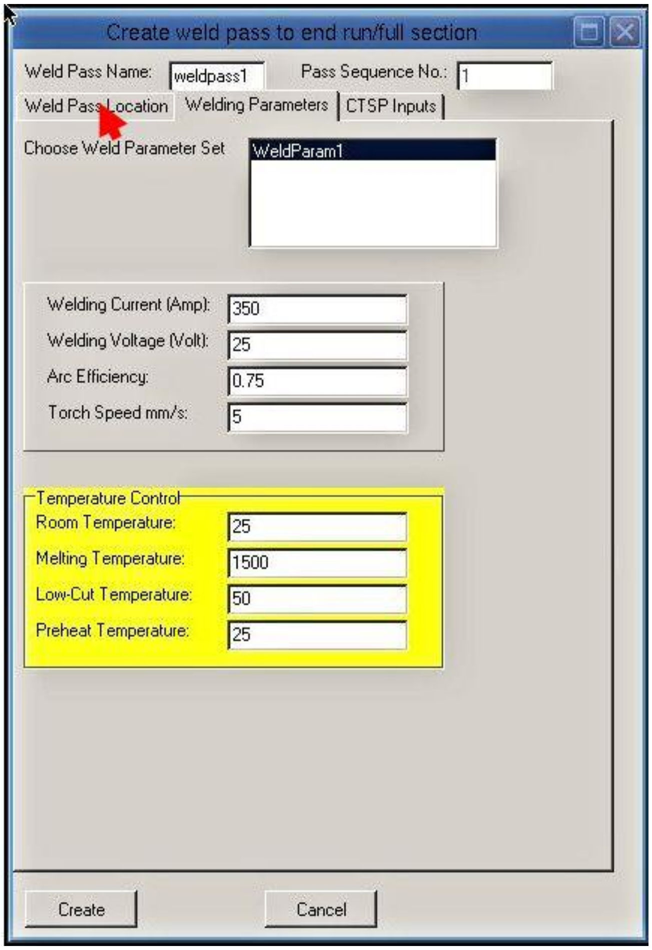


Figure 18 Weld parameter definition box

After completing the 'Welding parameters' box click on the 'Weld Pass Location' button as seen with the red arrow in Figure 18. The box shown in Figure 19 appears. Here the user chooses the weld material set (here we chose material 316 stainless steel from the VFT library for isotropic hardening). Next the user chooses the color for visualization of this pass after the definition.

Next in the process the user defines the pass as illustrated in Figure 20. With the 'First item' clicked the user chooses one element on the face of the weld as seen in the lower right with the green element face highlighted. The element face at the end of the weld must be chosen. For some welds the element faces might be hidden from view. For this case the user uses the 'H' or 'Hide' feature (Figure 16) which is described in the next example. The user then clicks the 'Second' button as seen with the red arrow in Figure 20. Then the user clicks any element in the direction of the weld. The weld pass elements are then highlighted. Figure 21 shows that the user clicks 'Third' and 'Fourth' to define the plate normal. Clicking on the plate draws an arrow as seen here. Note that the order of the normal definitions must match the plate thickness definitions made in Figure 17.

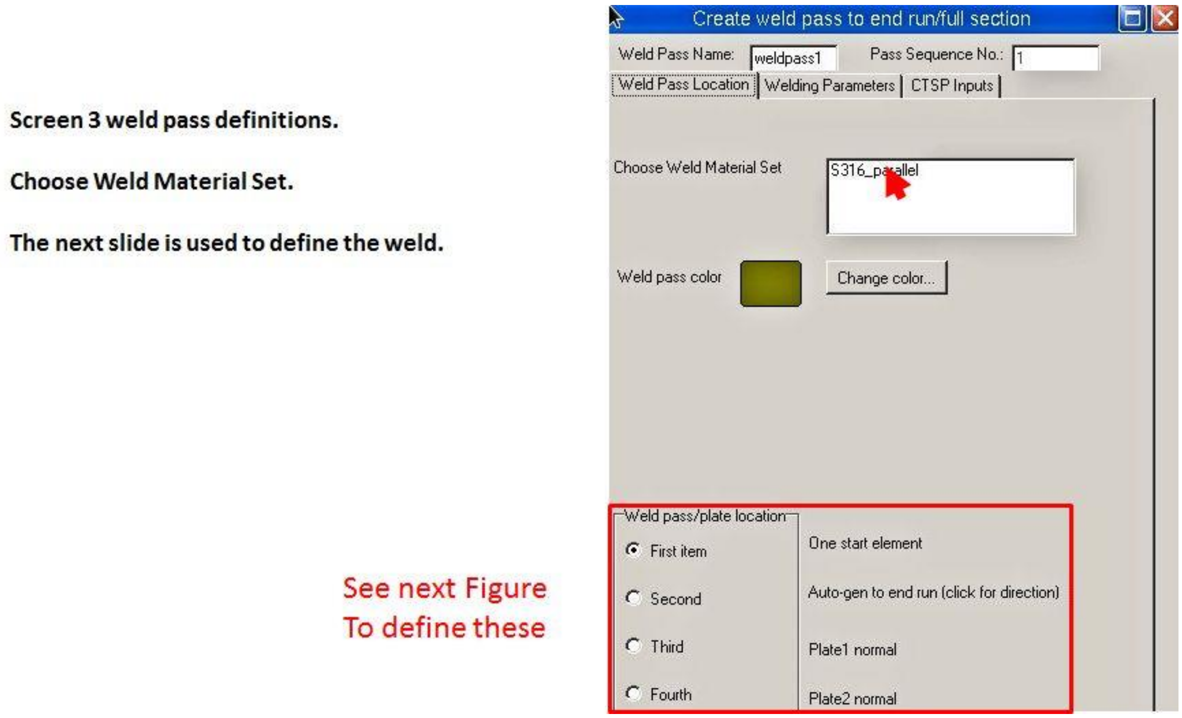


Figure 19 Weld pass and structural material definition box

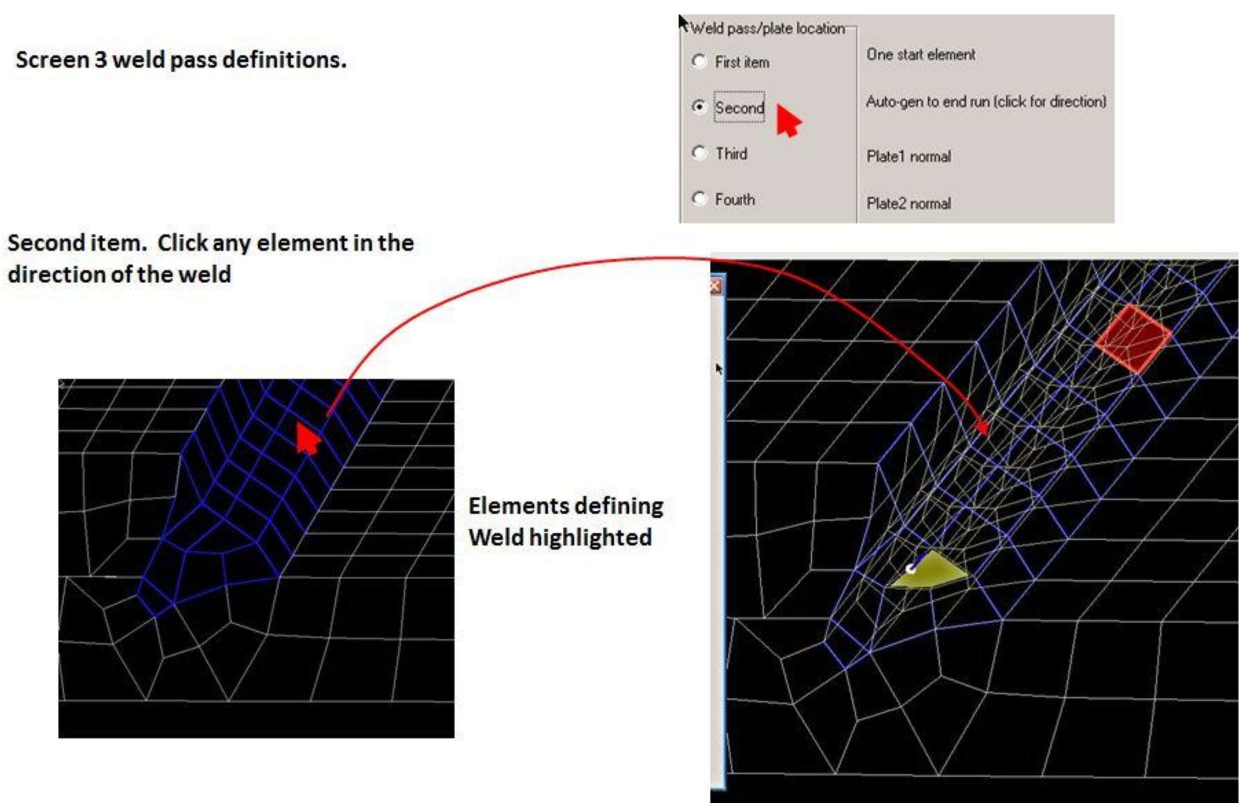


Figure 20 Defining the weld pass – Part 1

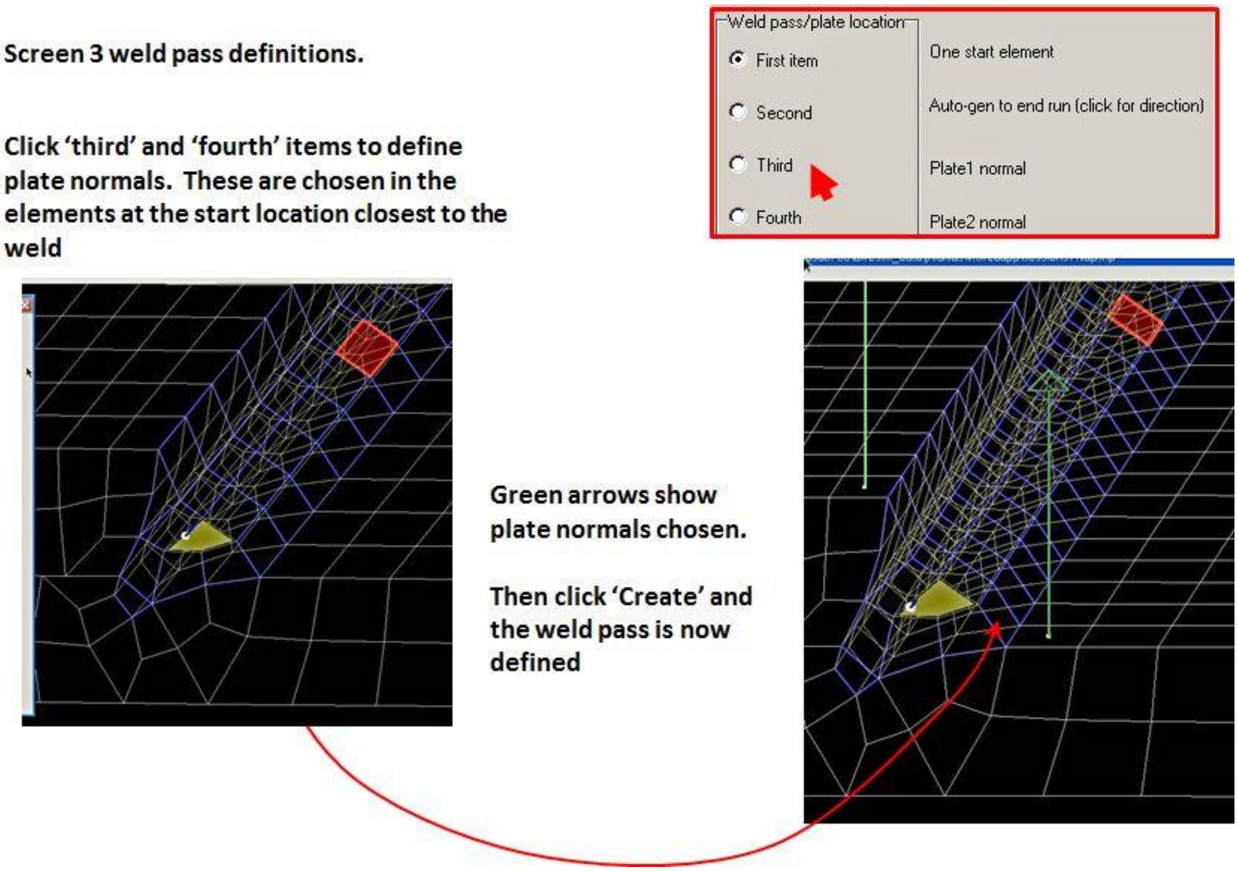
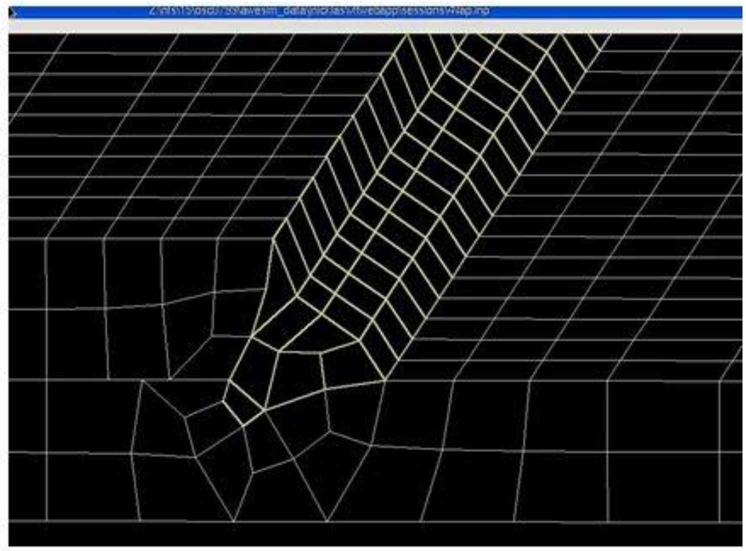


Figure 21 Defining the weld pass – Part 2

With the pass definitions provided, the user then clicks 'Create' and the pass is highlighted on the screen in the color chosen by the user as seen in Figure 22. The user then does this for all passes in the model. For this lap joint example there is only one pass so we are ready for the analysis. As also seen in Figure 22 it is recommended that the user save the VFTr model at this point so that it can be restarted later if desired. This is especially important for very large models where the user might define say 50 passes the first day and then start again the next day to complete the pass definitions. This is also useful for editing weld pass sequences, weld parameters, material properties, etc.

Go through the same procedure for every pass that must be defined.



It is also useful to save the VFT file in a format that can be re-opened later. Called 'Model.vftr' file.

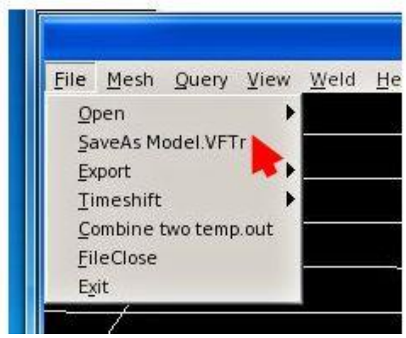
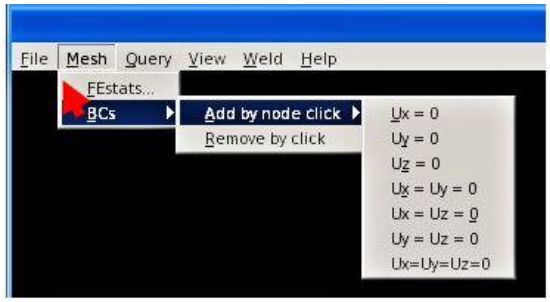


Figure 22 Completion of weld pass and saving of model

Step 4. *Define boundary conditions*. For computational weld modeling using VFT, users usually provide constraints that limit rigid body motion although many other types of boundary conditions might be of interest. The user can also provide a user defined set of boundary conditions. As seen in Figure 23 the user navigates to the 'Mesh' menu, 'BC' and then defined each boundary condition separately. The boundary conditions used for this lap example are shown in Figure 24. For problems where a large number of boundary conditions must be defined, or problems where a distortion control process like pre-camber will be used the user will likely define their own set of boundary conditions and then transfer this file to the working directory on OSC using the process discussed for the user material definition near the end of Step 2. The format for WARP3D boundary condition definition can be found in the WARP3D Manual which can be downloaded from the VFT site or from the WARP3D download site. However, it is useful to see the format for the cases where VFT defines boundary conditions for reference. For user definition of boundary conditions the file name must be defined as *.constraints, where * is the name of the WARP3D file (defined later) before transferring to the OSC analysis directory.

Go to mesh menu to define nodes with boundary conditions. For weld analyses this usually requires prevention of rigid body movement



To right is a node constrained in x and y.

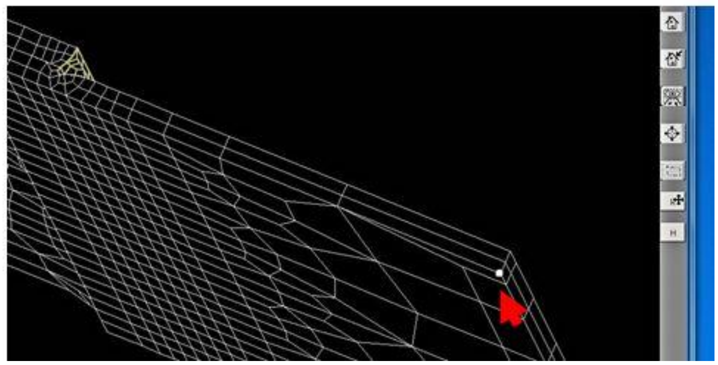


Figure 23 Defining boundary conditions

Go to mesh menu to define nodes with boundary conditions. For weld analyses this usually requires prevention of rigid body movement

Final BC for lap

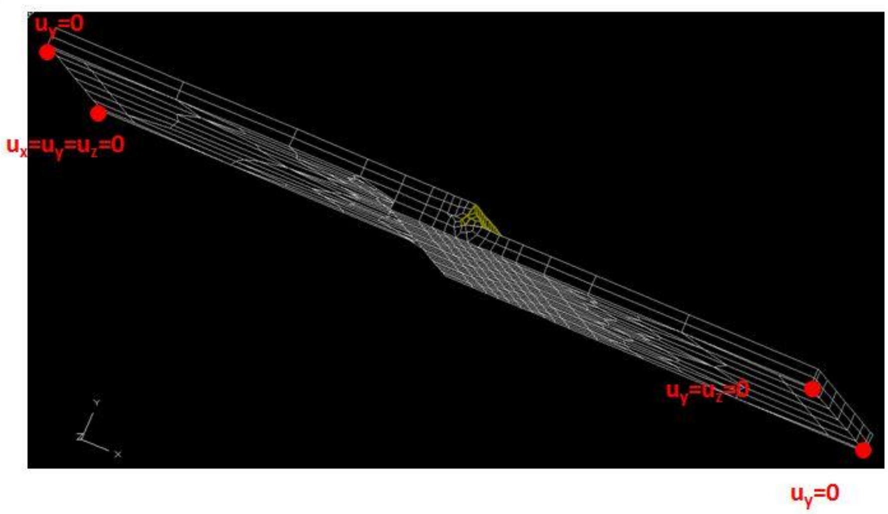


Figure 24 Defining boundary conditions for lap problem

Step 5. *Write out VFT solution input files*. Figure 25 illustrates how the VFT files for thermal solution (CTSP files) and structural solution (WARP3D files) are exported to enable the VFT solution to proceed. The user need not know the contents of these files. However, the advanced user may make changes directly to these files by examining them using the 'Files' menu.

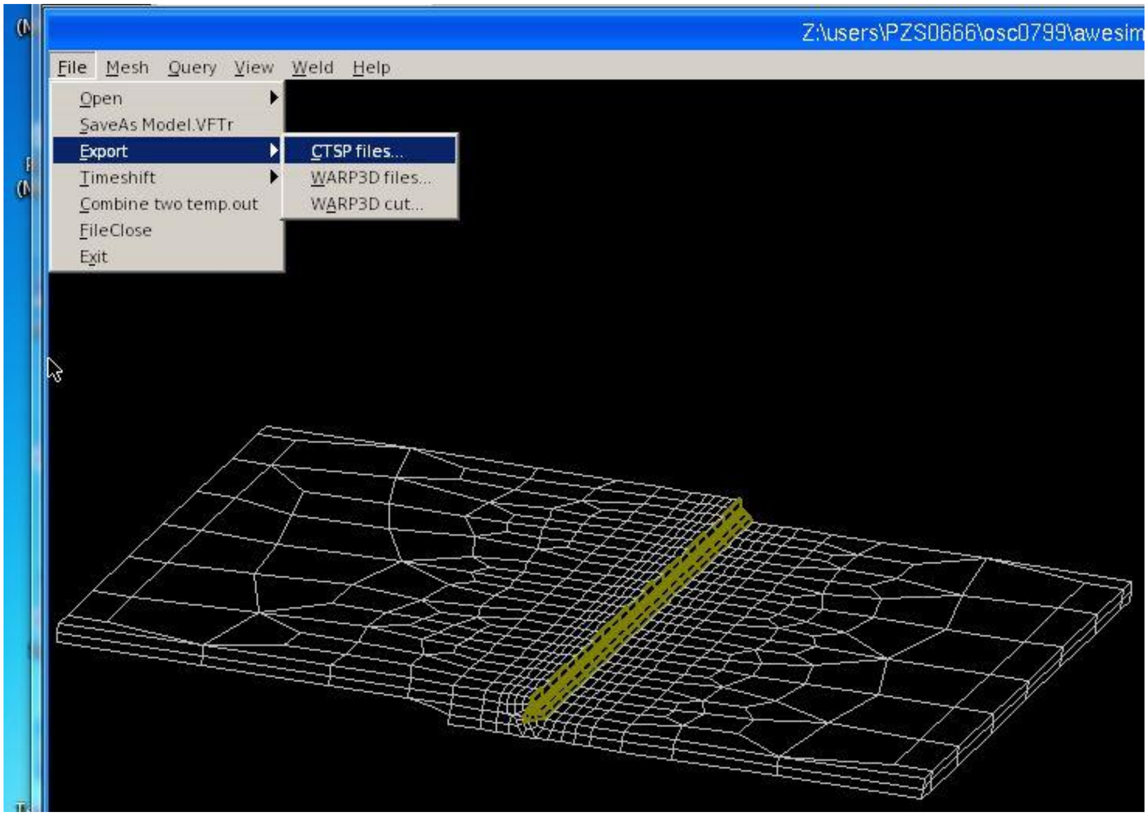


Figure 25 Writing out VFT files for solution

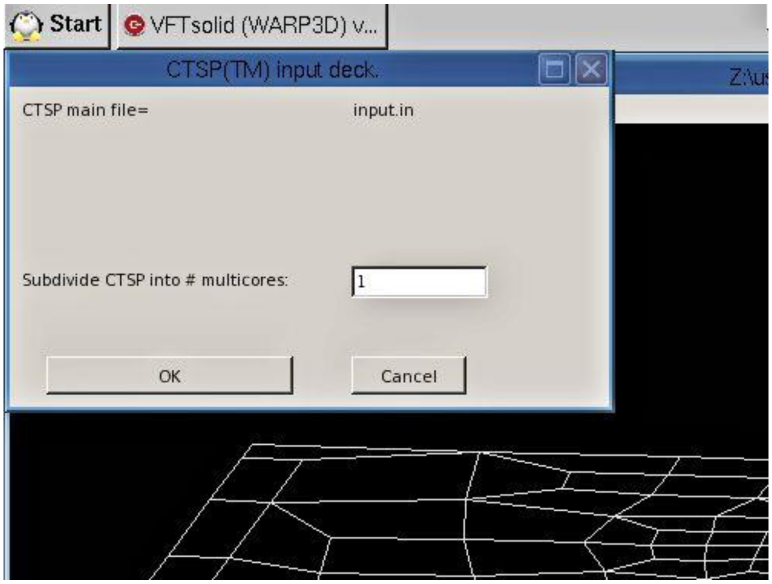


Figure 26 Writing out CTSP files for solution and choosing number of solution cores

The screen shown in Figure 26 appears when the user writes out the CTSP files for solution. The user is asked for the number of cores for solution. The user is prompted to click the 'OK' button prior to writing out the files to ensure that there were no errors. The user can choose as many cores as desired as long as the number of cores is not larger than the number of welds. The thermal solution is extremely fast. Next the user writes out the WARP3D files as seen in the process in Figure 27

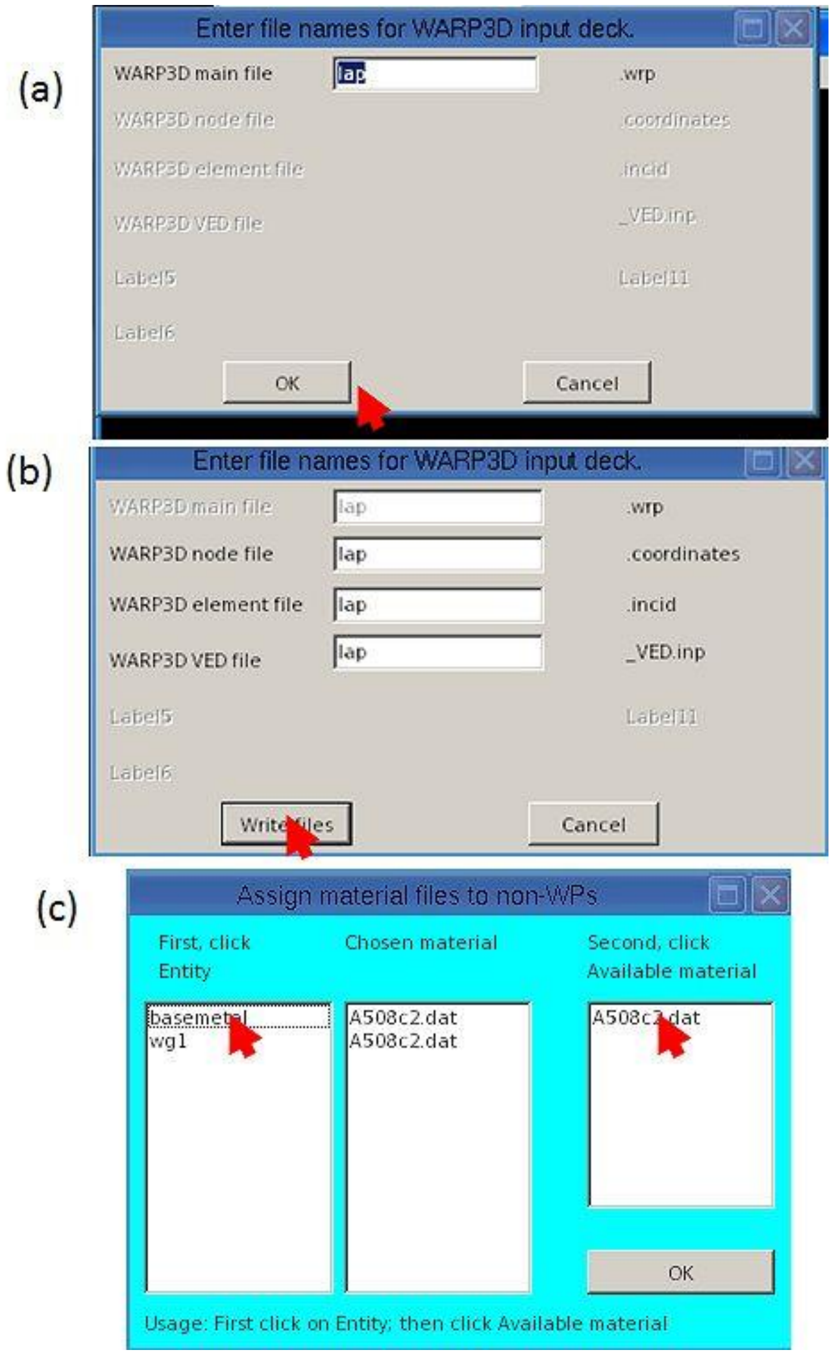


Figure 27 Writing out WARP3D files and choosing materials for each group

The screen in Figure 27 (a) first appears and the user defines a file name for solution. Here we name the files 'lap' for lap joint analysis. After clicking 'OK' the screen in Figure 27(b) appears. This represents the files that will be written in the solution directory that will be used by WARP3D. The files are:

- lap.wrp - this is the control WARP3D file and contains everything needed for WARP3D solution
- lap.coordinates – this is the file with nodes
- lap.incid – this is the file with element incidences (or finite elements in usual notation)
- lap_VED.inp – this is the virtual element detection (VED) file used to control elements ahead of the moving weld arc that have not yet been deposited (see VFT UMAT manual)

After clicking 'OK' to the screen in Figure 27 (b) the screen in c) appears. If the user clicks 'OK' without doing anything else these will be the material definitions for the analysis. The GUI creates a 'basemetal' element group by default (if the user has not defined other element groups in the *.inp file first read into the GUI). Alternatively, the user can define different materials for the different element groups if there are multiple materials in the model. This is done by first clicking and highlighting 'basemetal' then the material in the third column. Then the weld group 'wg1' may be clicked and the material defined. Since the weld pass element groups already had the material definition provided (Figure 19) it is normally not necessary to redefine the materials for the weld groups. This can be done for all element groups if desired.

Step 6. *Perform CTSP (thermal solution).* After writing out the files the solution is ready to proceed. The user clicks 'File-Exit' in the GUI then minimizes the GUI screen. Next the user goes back to the VFT browser control screen (Figure 28) and clicks 'Stop' as shown in upper illustration and Stage 2 appears (lower illustration). The user then clicks 'Launch' in the Stage 2 screen. The user then waits until the thermal solution is complete. Utility routines automatically write out temperature files necessary for visualization of the maximum temperatures for all welds and the maximum temperature for each individual pass.

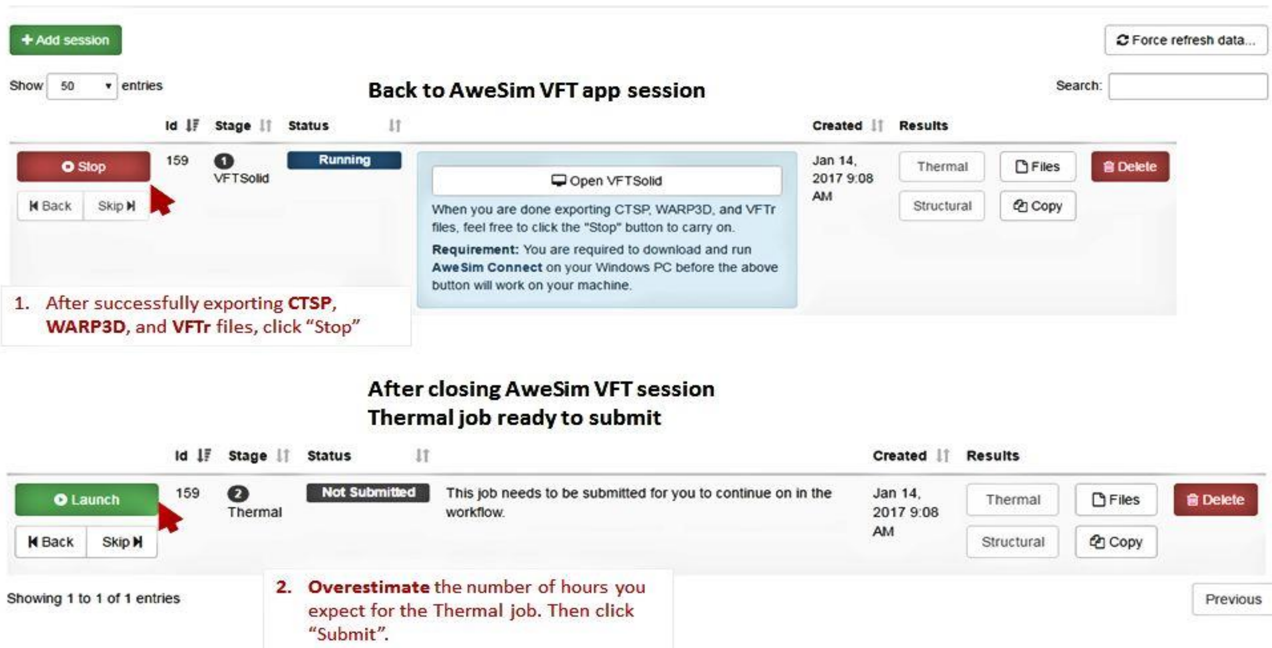


Figure 28 AweSim VFT app screen after closing GUI

After CTSP is complete the user usually wants to view the thermal profile to ensure that the fusion zone is properly captured. Referring to Figure 29, the user clicks on the ‘Thermal’ button and ParaView automatically opens so that the fusion zone can be viewed to ensure that the thermal solution is correct. If the fusion zone is not matched the weld parameters need to be changed and the solution run again.

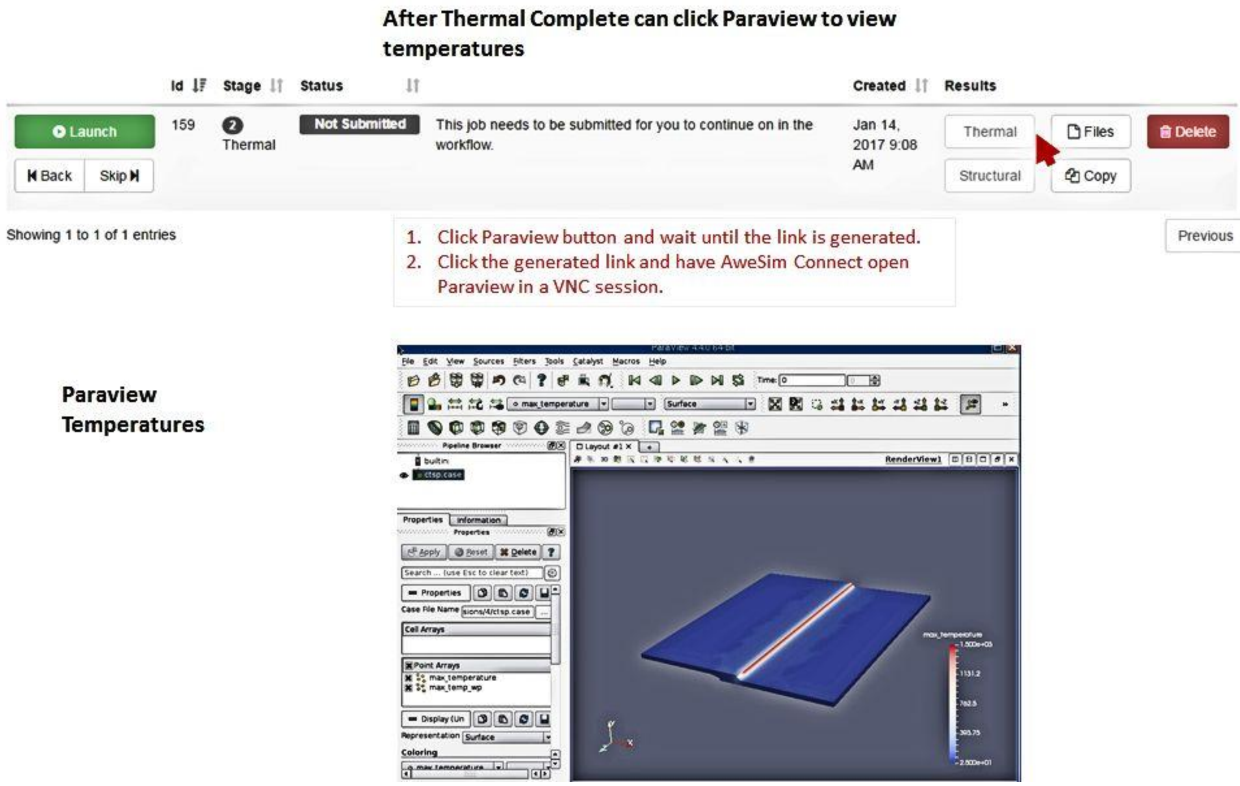


Figure 29 Visualization of temperatures with ParaView

Step 7. *Perform WARP3D solution.* After completion of the thermal solution in Stage 2 (and the user is satisfied with the thermal profiles created) the user then clicks on the ‘Launch’ Structural solution (Stage 3) seen in the top illustration in Figure 30. After clicking launch the VFT/WARP3D solution control parameters screen appears as seen in Figure 31. These parameters are described in detail in the VFT Solutions with WARP3D download discussed above. Here we provide a brief summary of these parameters.

At the top the user chooses the Wall time in hours that they estimate the structural solution will take on 20 processors (default on the super computer at present). If the user underestimates the amount of time required they can simply restart the solution from the point where the solution was stopped. The next parameter in Figure 31 is the Max total WARP3D thermal load steps. By default this is 10,000 which should suffice for most problems. This number can be up to 100,000. The ‘Restart thermal profile steps’ parameter represents the number of thermal profiles between saving of restart steps. For large problems these restart files can be large. The ‘Output thermal profile steps’ represents the number of thermal profiles between saving output results for visualization with ParaView after solution. Finally, N1, N2, N3 represent solution control parameters described in the VFT Solutions with WARP3D download. These are set at N1/N2/N3 = 1/2/2 by default and these parameter work for many problems. For some very fine meshes these parameters may be increased possibly increasing solution time. If divergence occurs during solution the user will restart the solution and increase these numbers.

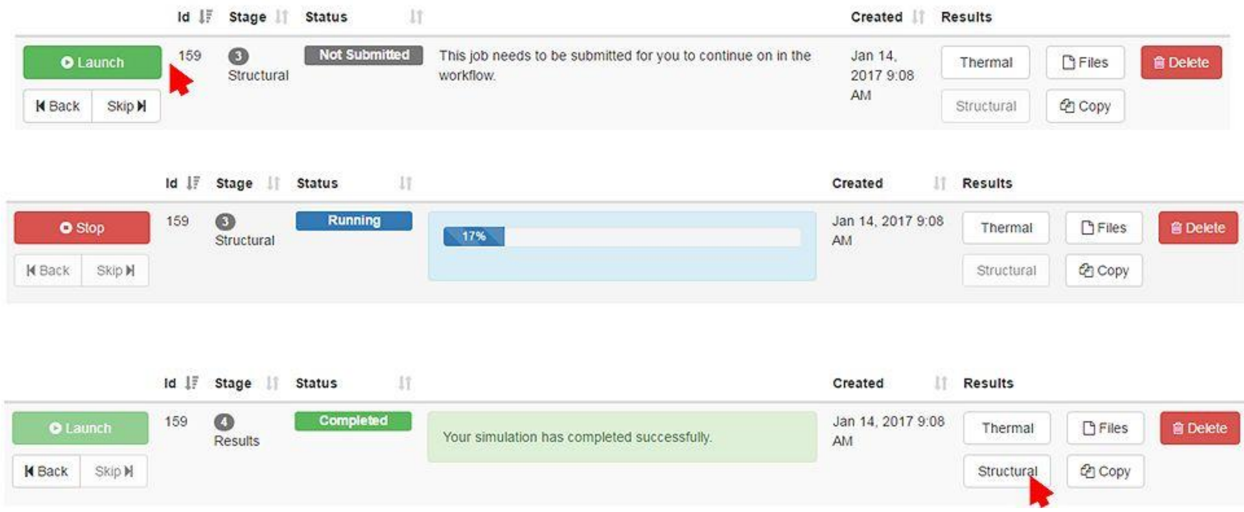


Figure 30 Launch Structural (Stage 3) solution and visualization

After launching the structural solution the screen in the middle of Figure 30 appears (solution progress bar) letting the user know the progress of the solution. When the solution completes the bottom screen in Figure 30 appears letting the user know that Stage 3 has been completed and Stage 4, which is visualization of results, is now possible by clicking on the 'Structural' button as seen here. If the solution did not converge, or there were other problems, the screen will tell the user and the errors must be found and the problem rerun.

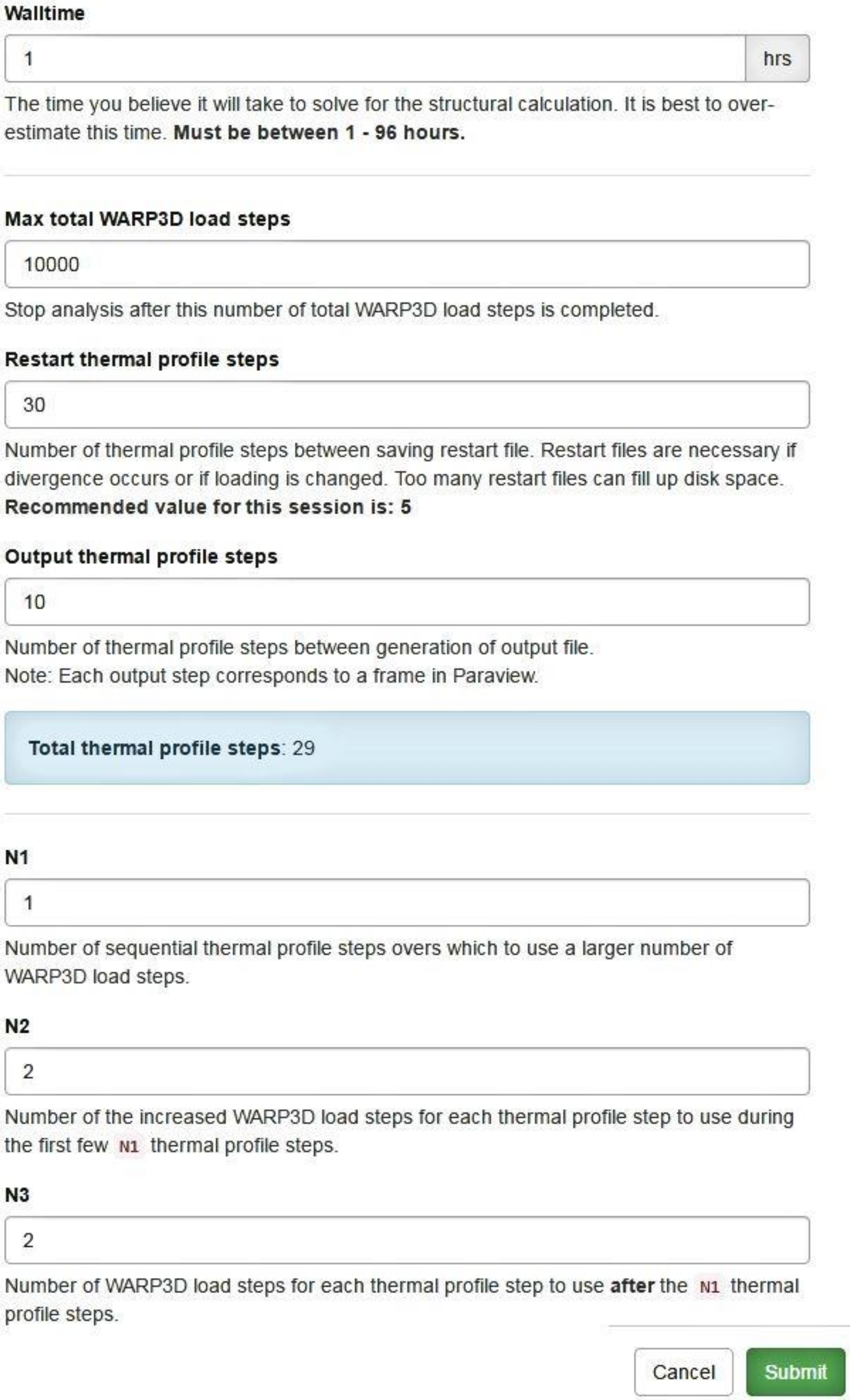


Figure 31 Warp3D solution control for VFT

Utility routines are automatically run (transparent to the user) to convert all WARP3D results to formats supported by ParaView.

Step 8. Invoke ParaView by clicking on the 'Structural' button in bottom screen in Figure 30. Weld residual stresses, distortions, strains, temperatures, etc., can be visualized.

Step 9. Determine if design or distortion goals are met and perform service life assessments as needed (fatigue, corrosion). If not, there are a number of strategies to remedy this situation. Invoke solution by rerunning the analysis with the changes specified. Methods for controlling distortions and weld residual stresses, and methods for performing corrosion, fatigue, and fracture stability can be found by downloading some of the publications in the VFT Documentation library.

4.4 Other Features in the GUI

There are a number of features of the VFT GUI which can also be used when defining a weld model. Refer to Figure 32. The 'Query' button can be used to query node and element numbers, determine distances and element face areas (for obtaining the size of a weld for instance). The 'View' button has the features shown in Figure 32 such as view orientations, background color, etc. The 'left' mouse button rotates the model, the 'right' button pans, and the 'wheel' modifies size also. The 'Weld' button is used to define weld parameters, materials, and create weld passes but also can be used to edit passes, delete passes, and modify weld sequences.

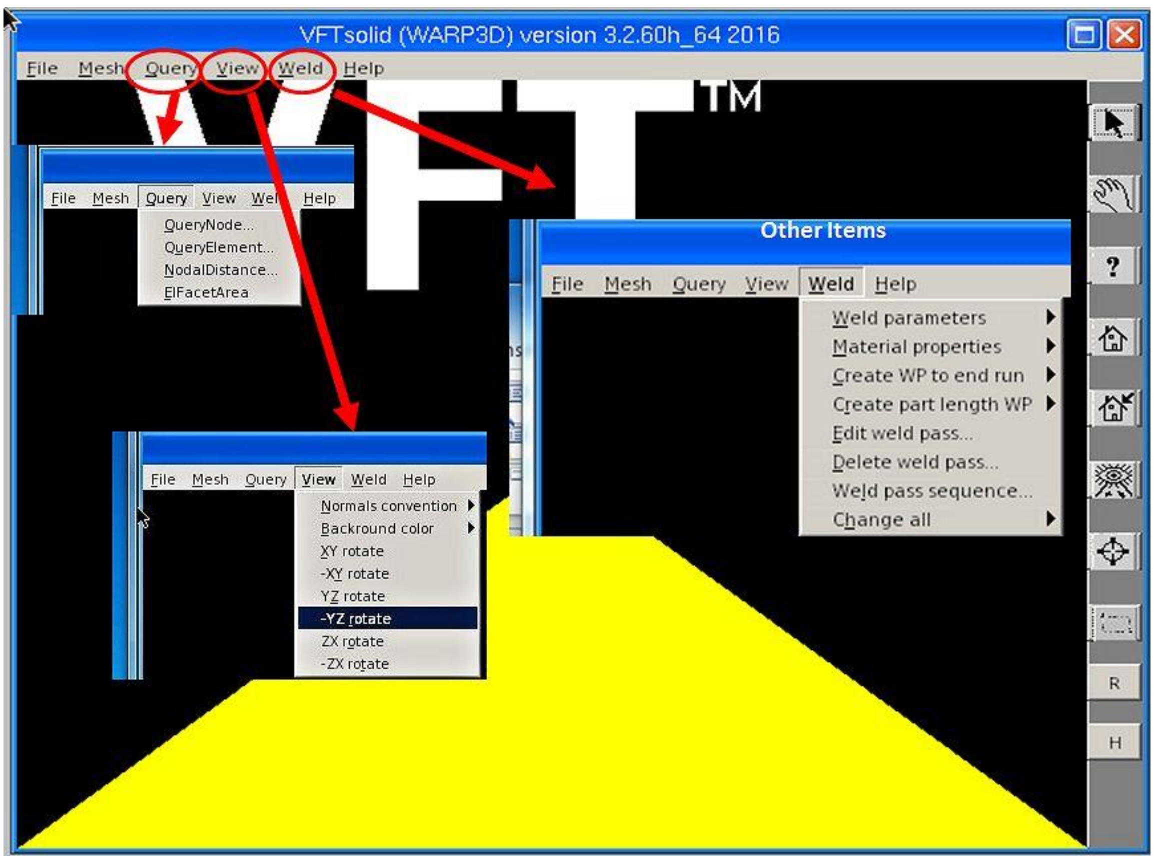


Figure 32 VFT GUI features

There are also convenient features for defining weld passes. Referring to the lap joint tutorial discussed in the prior section, the user can define part of the cross section as a weld. As seen in Figure 20 the lap joint example has 7 elements in the cross section. Referring to Figure 33 (upper left illustration) for the lap joint tutorial we chose 'Create WP to end run – Full section' when defining the weld for the tutorial. For this choice we only need to choose one element in the cross section as seen in Figure 20, choose the direction with the second click, and the entire cross section is picked for the weld.

However, by choosing 'Create WP to end run – Part section' (Figure 33 top) we can choose the elements in the cross section that we want to be part of this weld. As seen in the upper right of Figure 33 three elements were chosen and the weld pass is smaller than the entire cross section.

The user can also choose part length weld passes (bottom Figure 33). For this case (lower right in Figure 33) the stop location for the weld is chosen half way down the weld (orange highlights represent the pass). This option can also be performed with either Full or Part Section also.

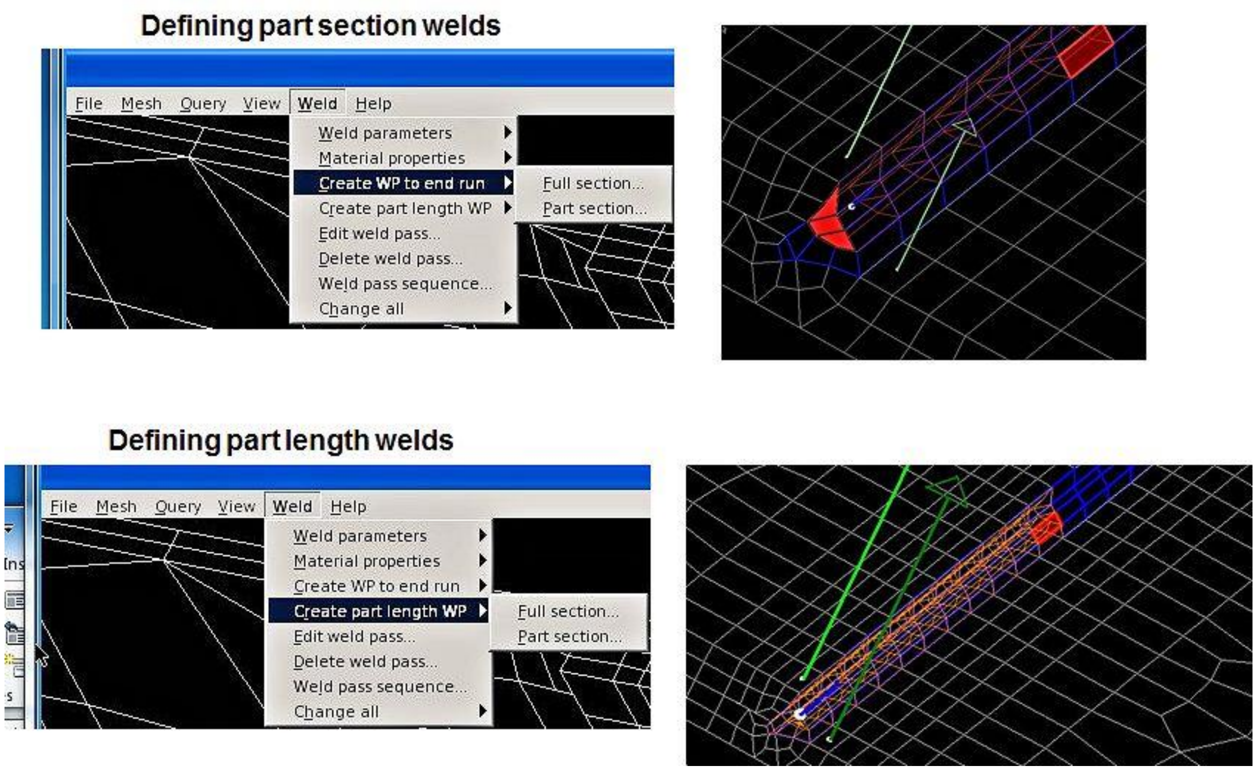


Figure 33 Defining part cross section weld groups and part length weld passes

Figure 34 also illustrates the features available in the GUI that are on the right side of the screen. In particular the 'R' (or Restore) and 'H' (Hide) buttons provide features to define weld passes that are hidden by other elements. This feature is discussed in the next tutorial problem.

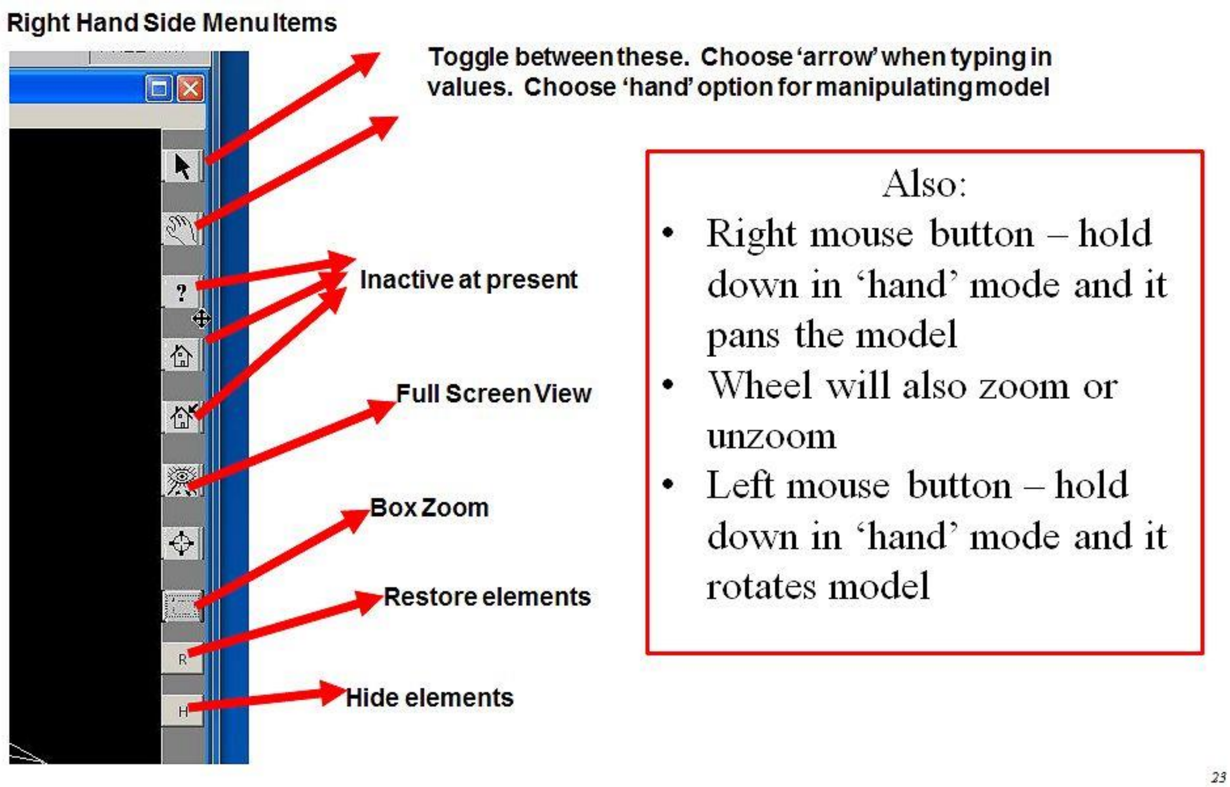


Figure 34 Other GUI features on right side of GUI screen

4.5 Submarine Tutorial Problem

A cylinder stiffened ring, which is a submarine segment, is seen in Figure 35. This consists of two fillet welds at the cylinder-ring intersection (dark and light green in Figure 35) and a Butt weld connecting the cylinder ring (blue). This is a problem where it is not possible to choose the element faces to define the weld so the 'H' (hide feature) must be used.

Step 1. Download the Submarine mesh from Documentation-Examples from VFT AweSim. Open the VFT GUI and open 'sub.inp'. The mesh shown in Figure 35 is seen.

Step 2. Define weld parameters and materials (Weld-Weld Parameters and Weld-Material Properties). Choose weld parameters and material properties shown in Figure 36. For the structural material file choose the isotropic hardening model for A508 class 2 (A508c2.dat) from the material drop down list.

Step 3. Define the weld passes. This requires use of the 'H' menu on the right side of the GUI. Choose 'View-XY Rotate'. The model appears as in Figure 37 upper left. Click the 'H' button on lower right of GUI. Go to the top just to the right of the 'blue' butt weld and create the cut lines as seen in Figure 37 top right. This is done by left clicking the mouse to create each cut line. Then right click the mouse. The model is cut as seen in lower right. Note if the cut is not what you wanted then successively continue the cut procedure and it will incrementally remove more cut portions of the mesh until you are satisfied that the cut is proper. Hit 'R' or restore at any time to restart the cut process or to go to the original uncut model.

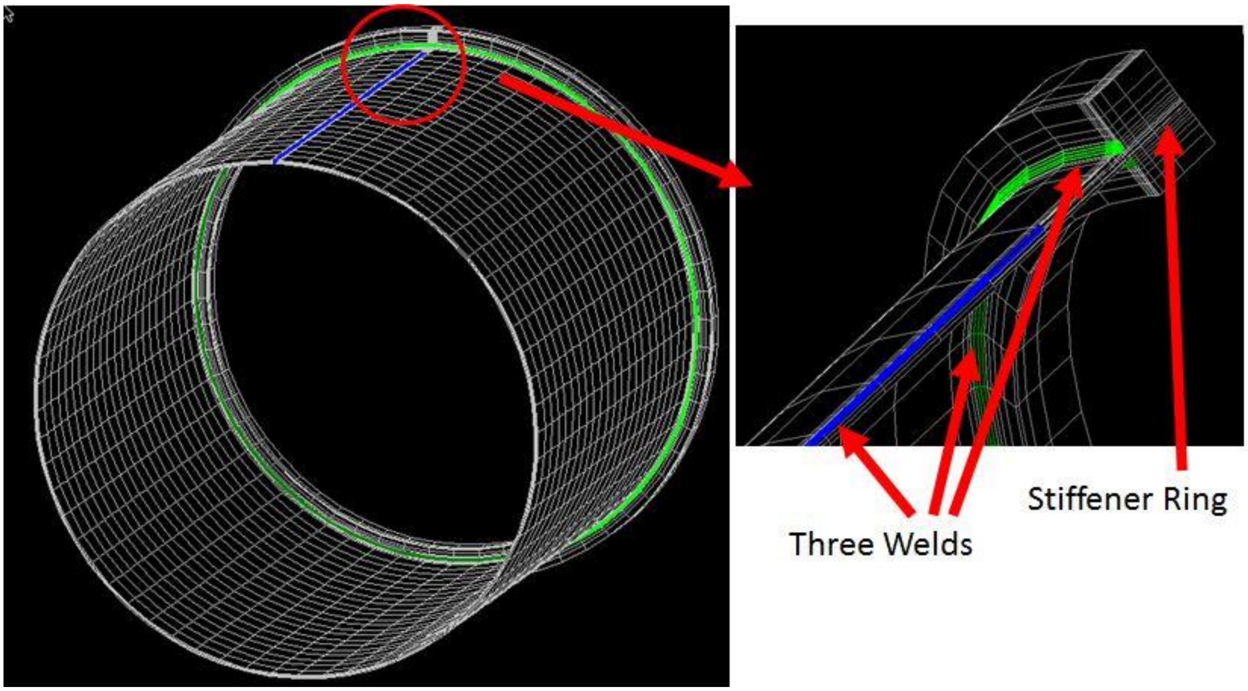


Figure 35 Submarine ring stiffened cylinder section tutorial

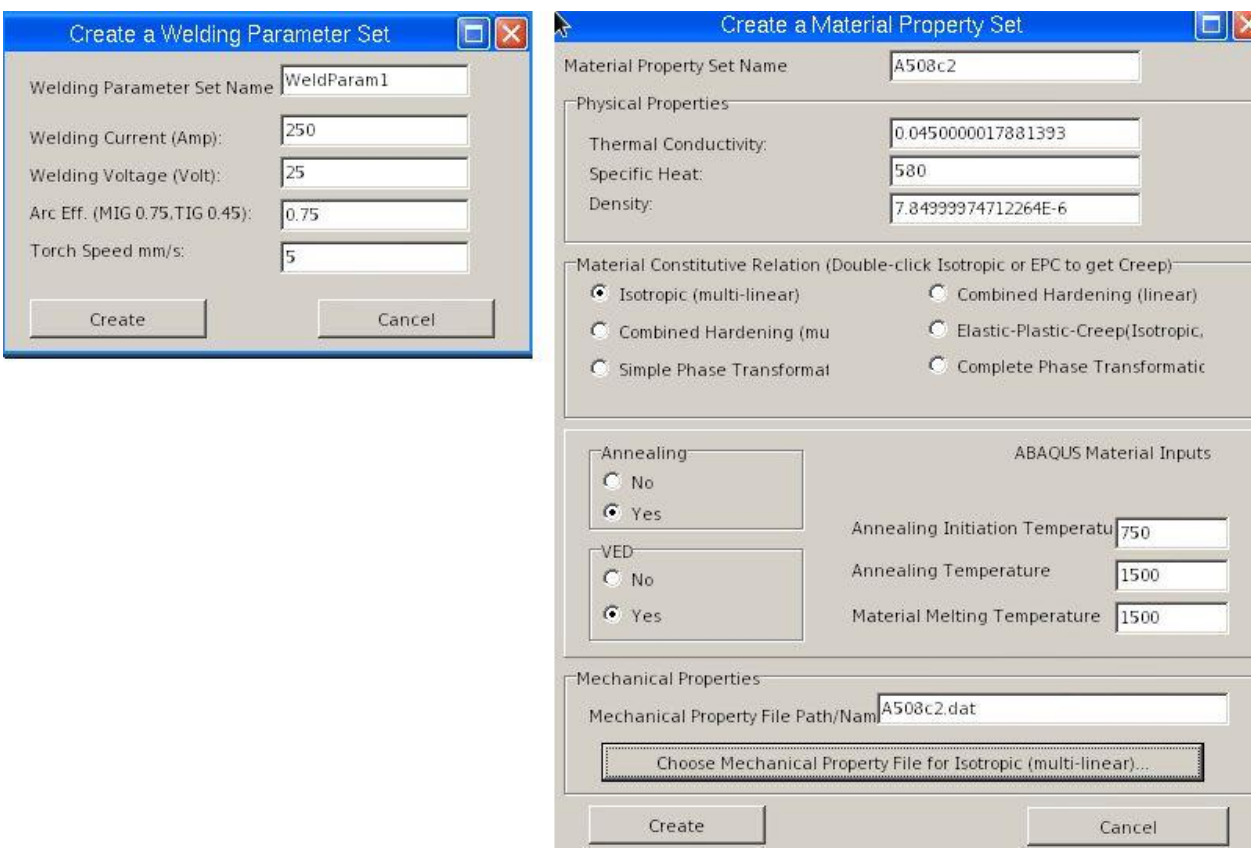


Figure 36 Submarine ring weld parameters and materials

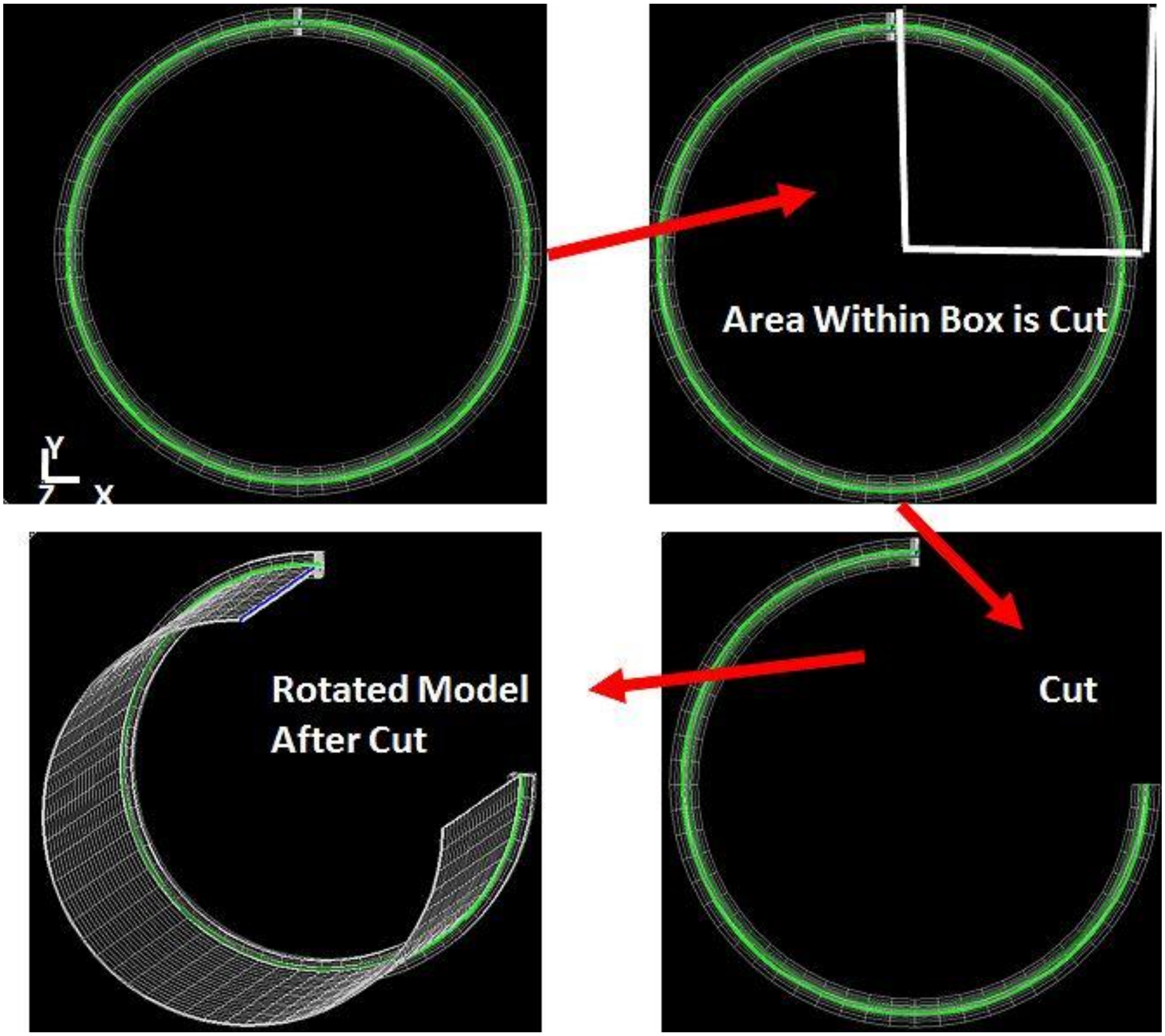


Figure 37 Cut procedure for submarine ring segment

Next define the weld passes on the cut model. We will do this here completely for illustration purposes. Rotate the model until the weld passes can be defined on the cut model. As seen in Figure 38 the user then chooses 'Create WP to end run-Full section'. The dialogue box shown in the left illustration in Figure 38 appears. The user fills this in. Here the weld type is T-Fillet, Joint Shape Non-Circular, Cool time 450 seconds and number of cooling steps 5. Next we choose the plate thickness. The cylinder thickness is 15.875 mm and the ring is 101.6 mm. The user then chooses the weld parameter box definition, then 'Weld Pass Location' box (bottom right Figure 38. Here we choose the weld material set as A508c2 and change the weld pass color to yellow as seen.

Next 'Weld Pass/Plate Location' parameters (bottom Figure 38). For this 'cut section' weld definition we first define the upper Tee-Fillet weld Figure 39 upper left. We choose 'First item' and click the face of the weld (Step 1 in Figure 39). The face is highlighted in yellow. Next we choose the weld direction (gray element identified in Step 2 of Figure 39). When this is clicked the blue arrow shows the weld direction chosen and all elements in this weld pass are outlined in yellow. We then choose the two plate normal (Step 3 and 4 in Figure 39). The plate normal is shown in green. The user should define these close to the start of the cross section for the weld. Note that the normal definitions must follow the same order at the Plate 1 and Plate thickness definitions in Figure 38. After this the user clicks 'Create' and the weld pass is shown (bottom left Figure 39).

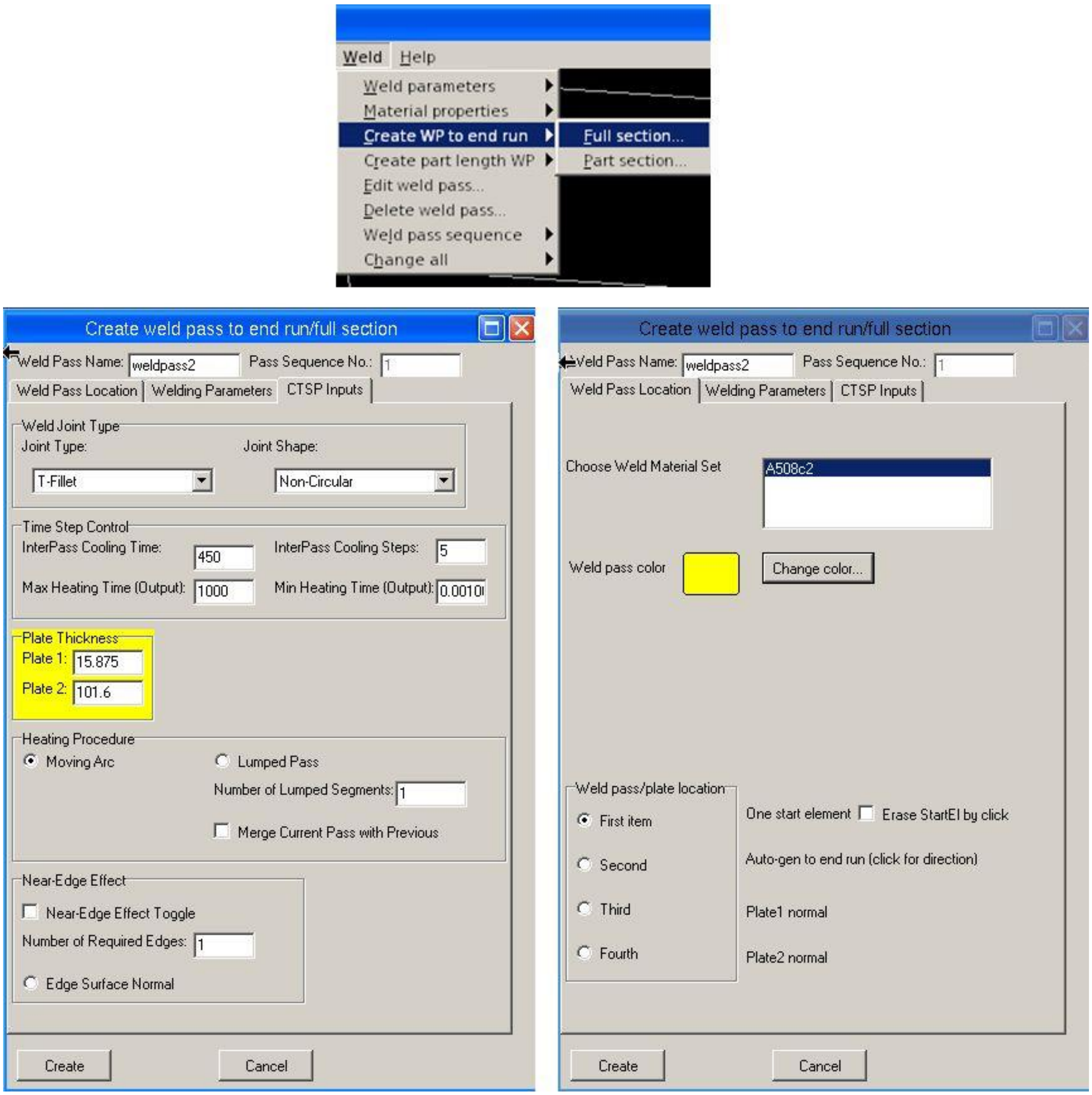


Figure 38 Weld pass definition procedure for submarine segment

The user then would rotate the model so that the fillet weld on the bottom can be defined. This rotation is necessary so that the normal can be properly defined.

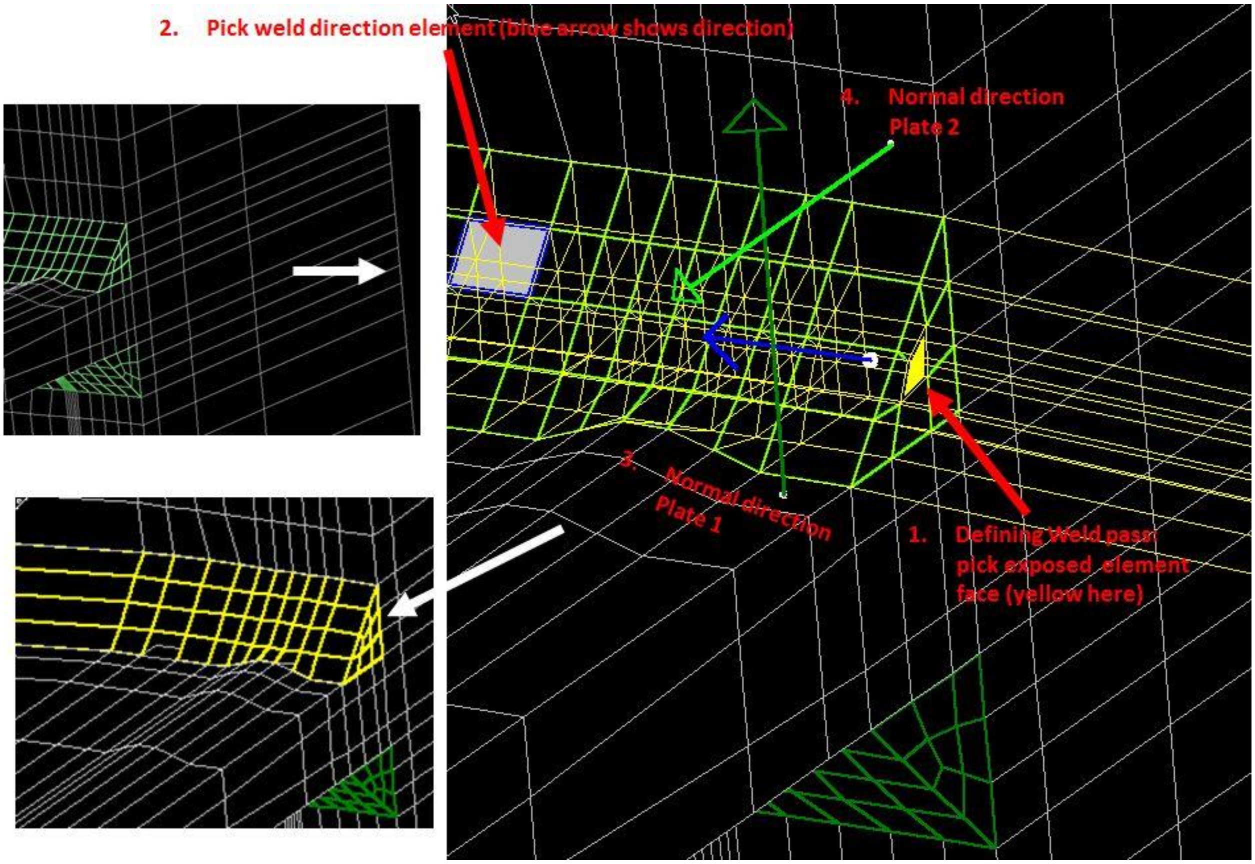


Figure 39 Choosing weld pass for Tee-Fillet weld in submarine

Next the third weld pass (the butt weld) is defined. The user would then click the 'R' button to restore the model to the no cut view first.

The user positions the model so that the butt weld can be defined (Figure 40 upper left and upper right). The user defines the CTSP input first. Remember to choose the Joint Type as V-Groove. Choose the cooling time to be a large number since this is the last pass and we want cool down to room temperature after this (here we chose 10,000 seconds). The plate thicknesses are both 15.875 mm for this weld. Next choose the material and weld color from the Weld Pass Location dialogue box. Here we chose orange for color. Then choose start element, direction, and the two plate normal (bottom right Figure 40). Click 'Create' and the weld pass is shown in Figure 40 lower left.

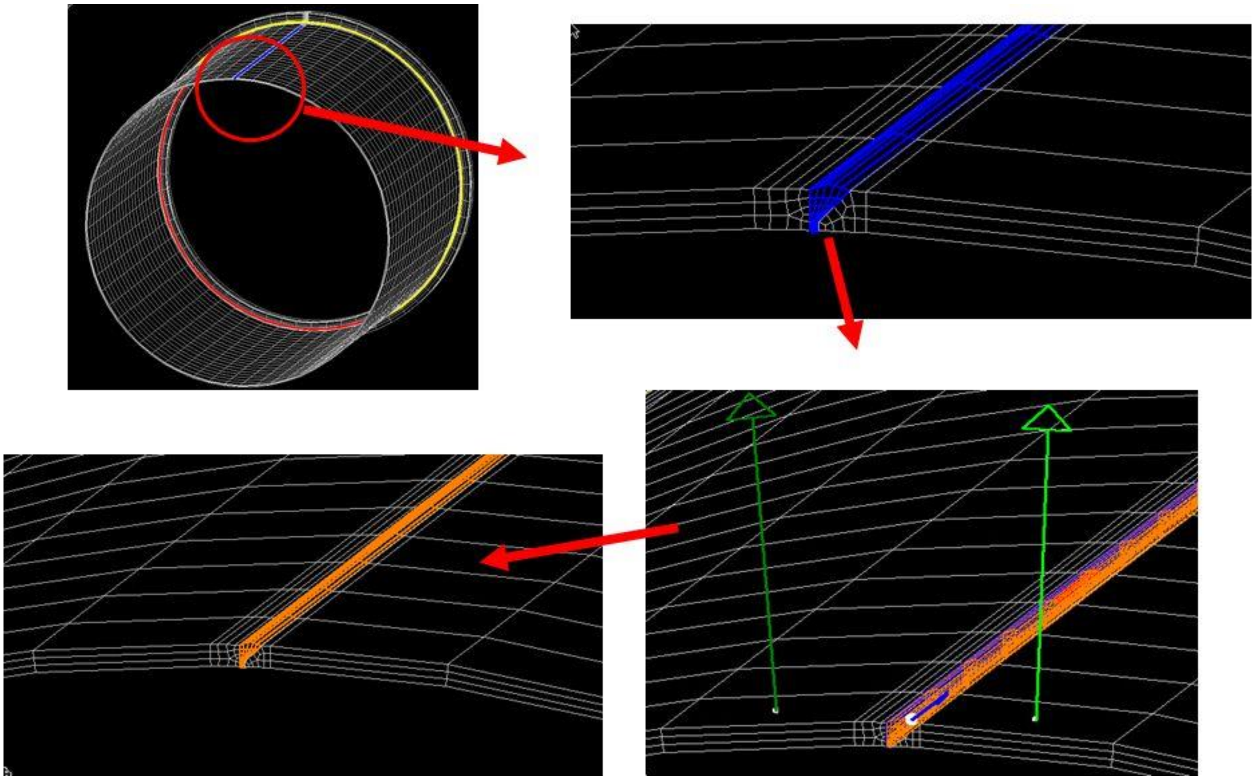


Figure 40 Choosing weld pass for butt weld in submarine

Step 4. Define the boundary conditions (Mesh-BCs-add by node click). Here we fixed points on the ring 90-degree away from the butt weld to have all degrees of freedom fixed. The user may want to explore other boundary conditions.

Step 5. Write out the input files for thermal solution (File-export-CTSP files). We chose 3 cores since there were 3 welds here. Also write out the WARP3D files (File-export-Warp3D files). Choose 'sub' for WARP3D main file name. When the material definition box appears (Figure 41) the user clicks on 'basemetal' in first entry and then 'A508c2.dat' in the second column on the right. Note that VFT assumes that all material that is not in a weld is 'basemetal' unless element groups for other plates were explicitly defined in the original input file. The three weld passes here have already had their weld material definitions defined. Do not forget to save the model as a 'VFTr' file. Then click 'File-Exit' and go to the VFT browser window again and click the red 'Stop' button to complete Stage 1.

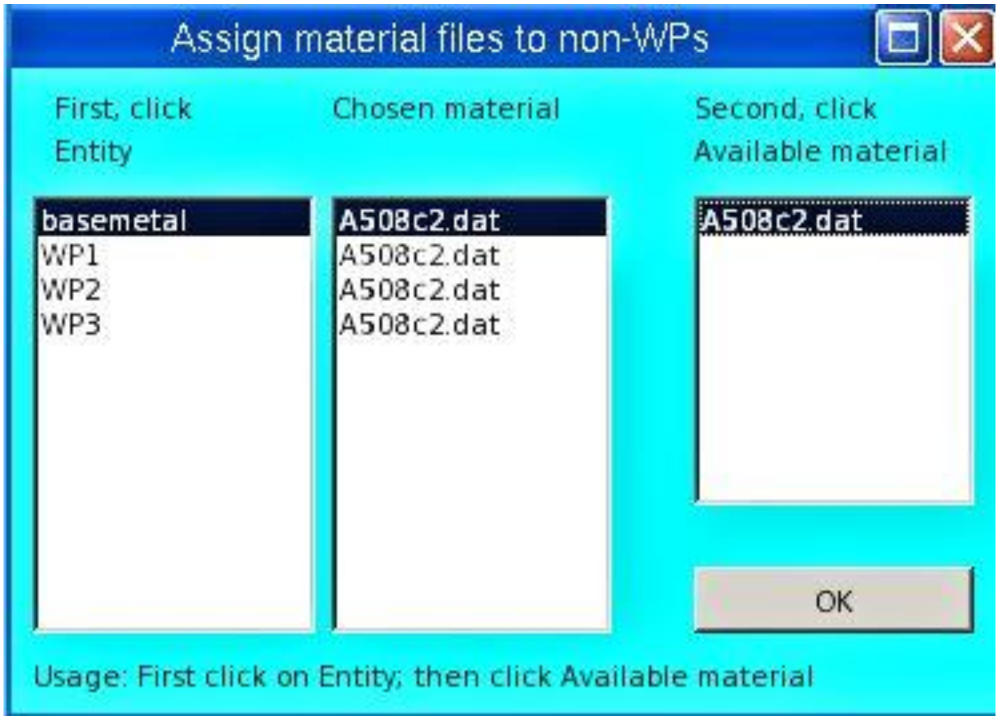


Figure 41 Material definition box for submarine model

Prior to Step 6 the user may want to examine the files that were produced by the GUI. This is done by clicking on the 'Files' button. This takes the user via WinSCP to the corresponding directory where this analysis is being performed on the OSC supercomputer. These files are described in the fourth set in the training materials section which can be downloaded (Section 4.1). For the submarine problem, a snap shot of this directory is shown in Figure 42. The three CTSP subdirectories (CTSPsubd001 to 003) are for each core the thermal solution will be run on. In these directories the 'input.in' file consists of the input file for solution of the thermal solution for that core. The definitions of all input parameters can be found in the CTSP manual. In particular, examining the first few lines of input.in CTSPsubd001 (Core 1 – files can be viewed by clicking on them which invokes the editor). Figure 43 Input file (input.in) in Core 1 (first few lines). See CTSP manual. Figure 43 shows the first few lines of the Core 1 input.in file. The red circle in Figure 43 represents the power input (Amps times Volts). Recall from Step 3 (Figure 36) we defined Amp=250, Volts = 25 for power input 6250 as seen. If the fusion zone is not properly matched the thermal solution should be redone with modified weld parameters. This can be done by going into the GUI and redefining the parameters. Alternatively, the user can change this number in the input.in files for each pass and then re-run CTSP. This is typically done for advanced users since it is fast.

The other files in the directory (Figure 42) consist of the WARP3D input file (sub.wrp) and are described in the files and WARP3D summary slides for the interested user.

Step 6. The next step is to launch the thermal solution in Stage 2 by clicking on the green 'Launch' button. This performs the analysis on each core, merges results, and writes out files that can be visualized in ParaView. The user can determine the progress of this solution by examining the 'Results' folder in Figure 42. CTSP solutions are very fast. The user will likely want to examine the predicted fusion zone by clicking on the 'Thermal' button in Stage 2. The ParaView screen will appear and the user clicks the green 'Apply' button. For these definitions the heat input may have been a little low so the user may want to redo the analysis. This is discussed later. Exit ParaView (Files-Exit) prior to running the WARP3D analysis in Stage 3.

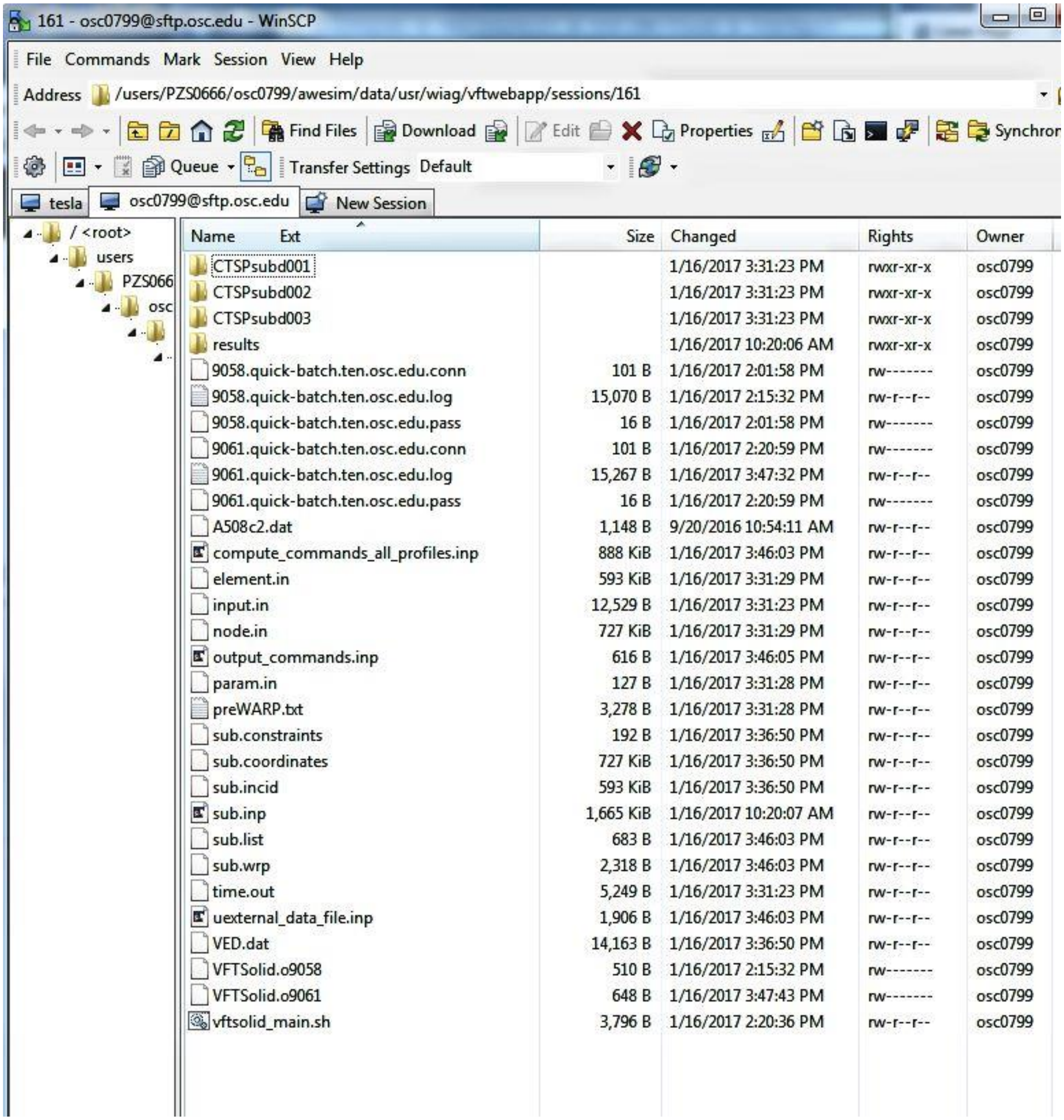


Figure 42 AweSim OSC directory for this submarine problem

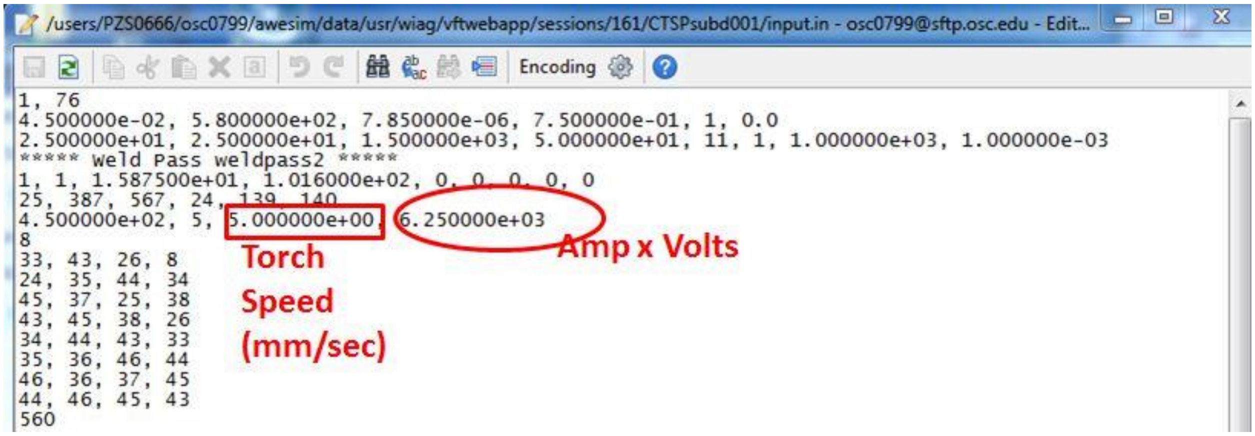


Figure 43 Input file (input.in) in Core 1 (first few lines). See CTSP manual.

Step 7. Launch structural WARP3D solution. Choose the 'Restart thermal profile steps' and 'Output thermal profile steps'. Here we chose 30 and 10 for these respectively.

Step 8. Click the 'Structural' button to observe results after solution is complete. The ParaView manual is provided for download so that the user can become familiar with it.

Step 9. Redo analysis if desired.

The format of some of the files used for the submarine problem are summarized in Section 5. Figure 58 shows the format of the uexternal_data_file.inp shown in Figure 42 while Figure 60 shows the format of the WARP3D input file for the submarine problem discussed in Section 4.5. Discussion of some of these other files are also shown in Section 5.

4.5.1 Modify Thermal Solution for Submarine Model

The fusion zone was a little small for the submarine using the weld parameters chosen (Amp=250, Volt=25). The user can redo the thermal solution several different ways.

- The user can click the 'Copy' button in the VFT AweSim browser access. This creates another session where the VFTSolid GUI can be launched. The user can then open the file as a 'VFTr' file (which the user saved) before closing the GUI. After solution the user will then have two session results both with different heat inputs for direct comparison.
- The user can click the 'Back' button in the original session. The first time take the user to Stage 3. Clicking 'Back' again takes the user to Stage 2 again. Note that the user could then run the thermal solution in Stage 2 or the structural solution in Stage 3 if desired again. Clicking 'Back' again takes the user to Stage 1. Here the user can launch the GUI and open the VFTr file and make changes as appropriate, and then go through the procedure again.
- The third was is an advanced VFT user feature. The user can open the 'input.in' files in the CTSP core subdirectories and make changes directly and redo the analysis. Here we briefly discuss this option.

4.5.2 Modify Thermal Solution by changing CTSP files directly

Referring to Figure 43 click 'Files' and open CTSPsubd001. Modify the weld power (Amps x Volts). Here we will change the power from 6250.0 To 10,000.0 in each core. This simply requires editing the file (Figure 43) and then saving for each core. After modifying the three files go back to Stage 2. Click 'Launch'. After completion examine the fusion zone by clicking the 'Thermal' button. The user will see that the temperatures are higher and the fusion zone is larger. The user then re-runs the Structural solution in Stage 3. The user should not change the torch speed since this affects other files (VED for instance) and should only be done by an expert. Note that this can also be done after the 'Copy' command in the second session. This technique should only be performed by the advanced user since problems can occur if this is not done properly.

4.6 Head Nozzle Tutorial Problem

This example model can be downloaded from the documentation VFT page (Head_nozzle). The model is shown in Figure 44 and Figure 45. This is a narrow gap weld with a very coarse weld pass mesh. Even with this coarse mesh the results are reasonable. The nine solution steps are briefly discussed.

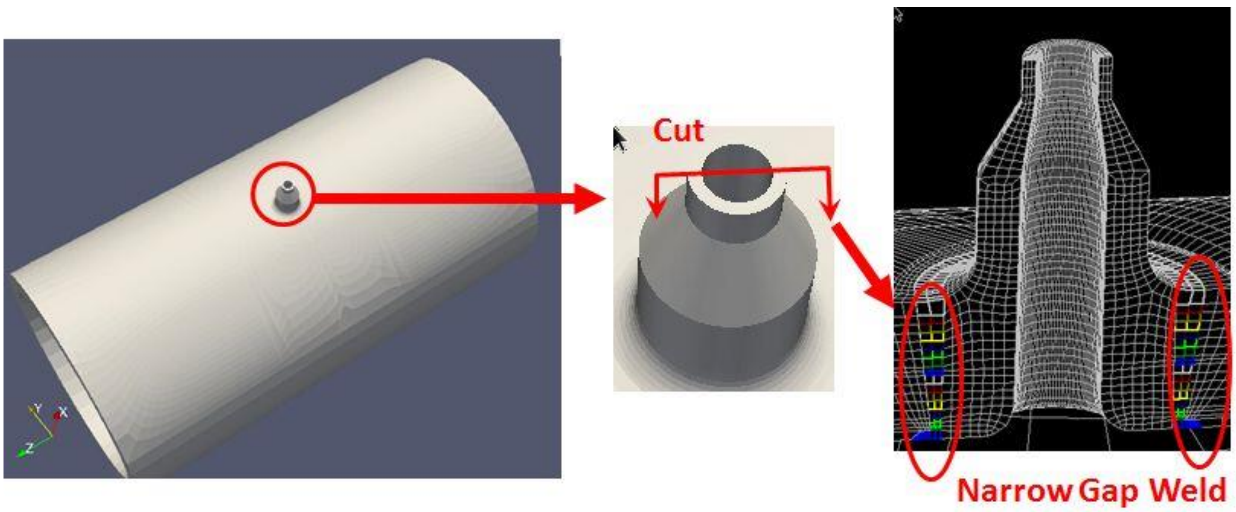


Figure 44 Head nozzle model (colors on right indicate weld passes

Step 1. Read the model into the VFT GUI. Use the 'H' (hide) feature to reveal the weld passes (Figure 46). It may require several successive applications of this to achieve the cut of interest. The 'red' line shows where the cut was made (Figure 46). The "Hide" feature was used, then further used consecutively until achieving the desired cut. Note that the user starts by pushing down on the left mouse button and creating a line. After that the user can pull the mouse to new locations and continue clicking until complete. Clicking right mouse button invokes the 'Hide' feature each time.

Step 2. Create weld parameter set. Choose Amp=350, Volts=25, torch speed 5 mm/sec, and arc efficiency (MIG) = 0.75. We recommend that the user try other parameters to observe the differences in fusion zone prediction. Create material definition sets. Here two materials were chosen, one for the weld metal (Alloy 182 isotropic hardening) and another for the nozzle and piping (316L stainless with combined mixed hardening). Keep thermal physical properties at the default.

Step 3. Define the weld passes. Rotate the model so that the cut face is visible with the weld passes for this narrow gap groove weld. Click 'Weld-Create WP to end run-Full Section'. The 'CTSP Inputs' box appears (Figure 47). Choose 'V-Groove', wall thickness of 101.6 mm for both sides. The user can determine the thickness of each side by using the 'Query-Node Distance' menu item. Click 'Weld Parameters' box and choose. Then click 'Weld Pass Location' tab

(Figure 47 lower left). The pass color is chosen as red and weld pass material as Alloy_182. The passes are then selected as in Figure 47 right. The user clicks on the 'First Item' or weld start element face and then along any line in the direction of the weld (Second Item yellow here). After clicking 'Second Item' the elements that were selected are highlighted in the chosen color (note that we chose red for this pass and Alloy_182 material). Then define the two normal directions on the base material to the left and right of the weld at the top of the nozzle weld area. After clicking the 'Create' button the pass is shown defined in red (bottom right Figure 47). The user does this for each of the 16 passes. For the other pass definitions the user does not need to redefine the normal on the 'Weld Pass Location' tab unless they want to. For the final pass choose a long cool down period (we chose 15,000 seconds here).

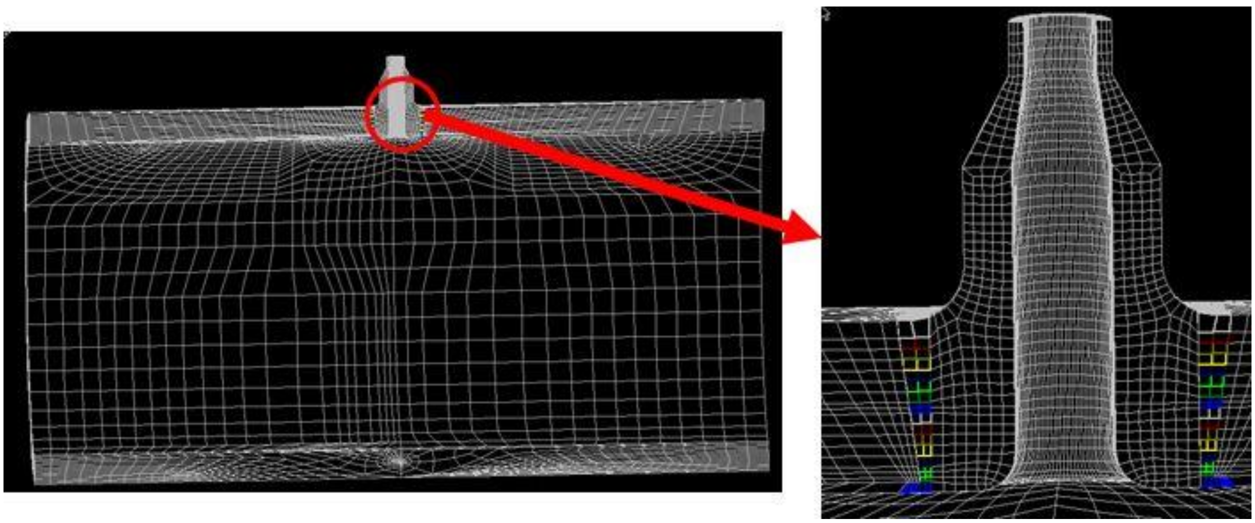


Figure 45 Head nozzle model (colors on right indicate weld passes

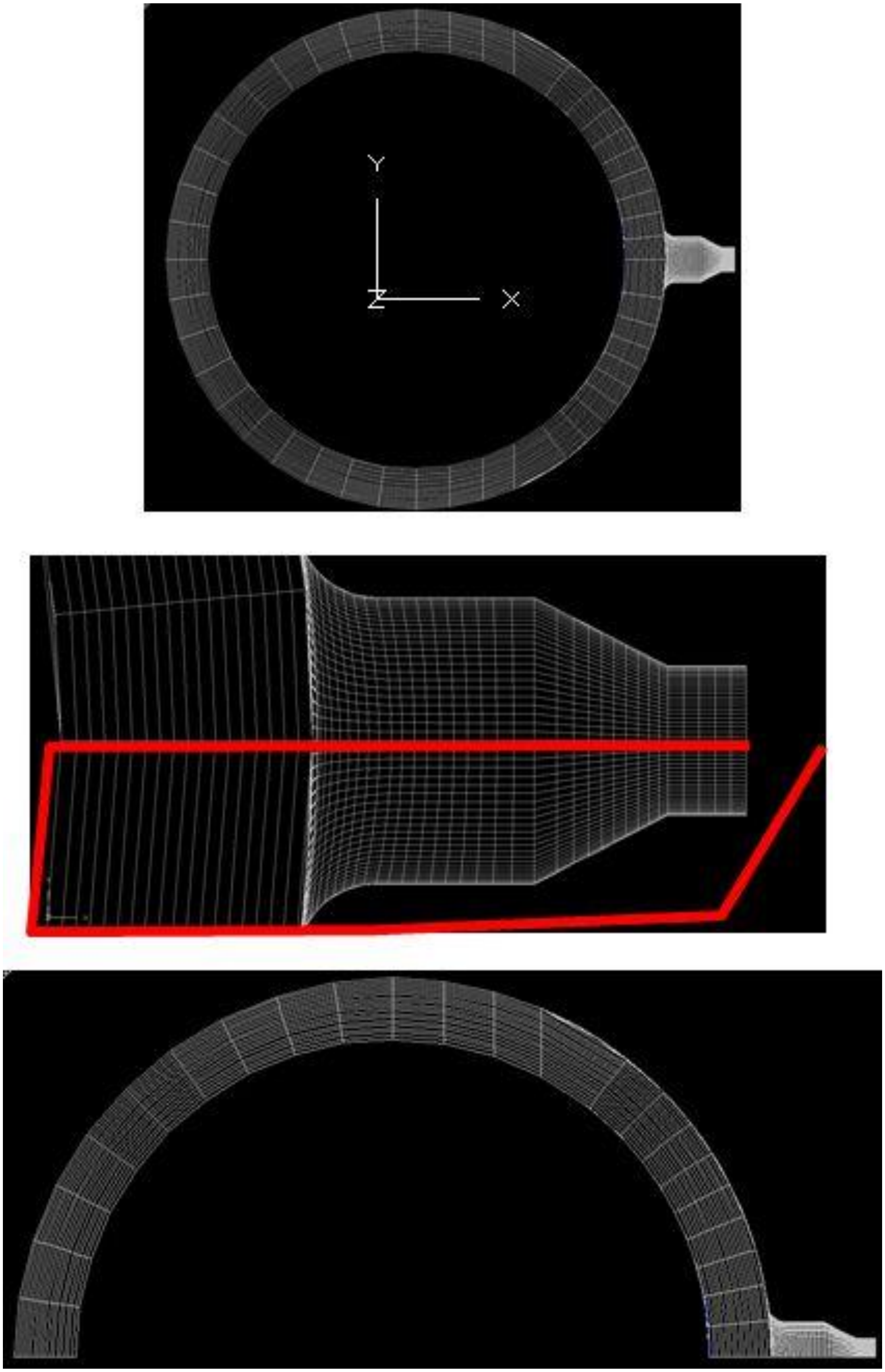


Figure 46 Use 'H' to hide elements to expose weld groups

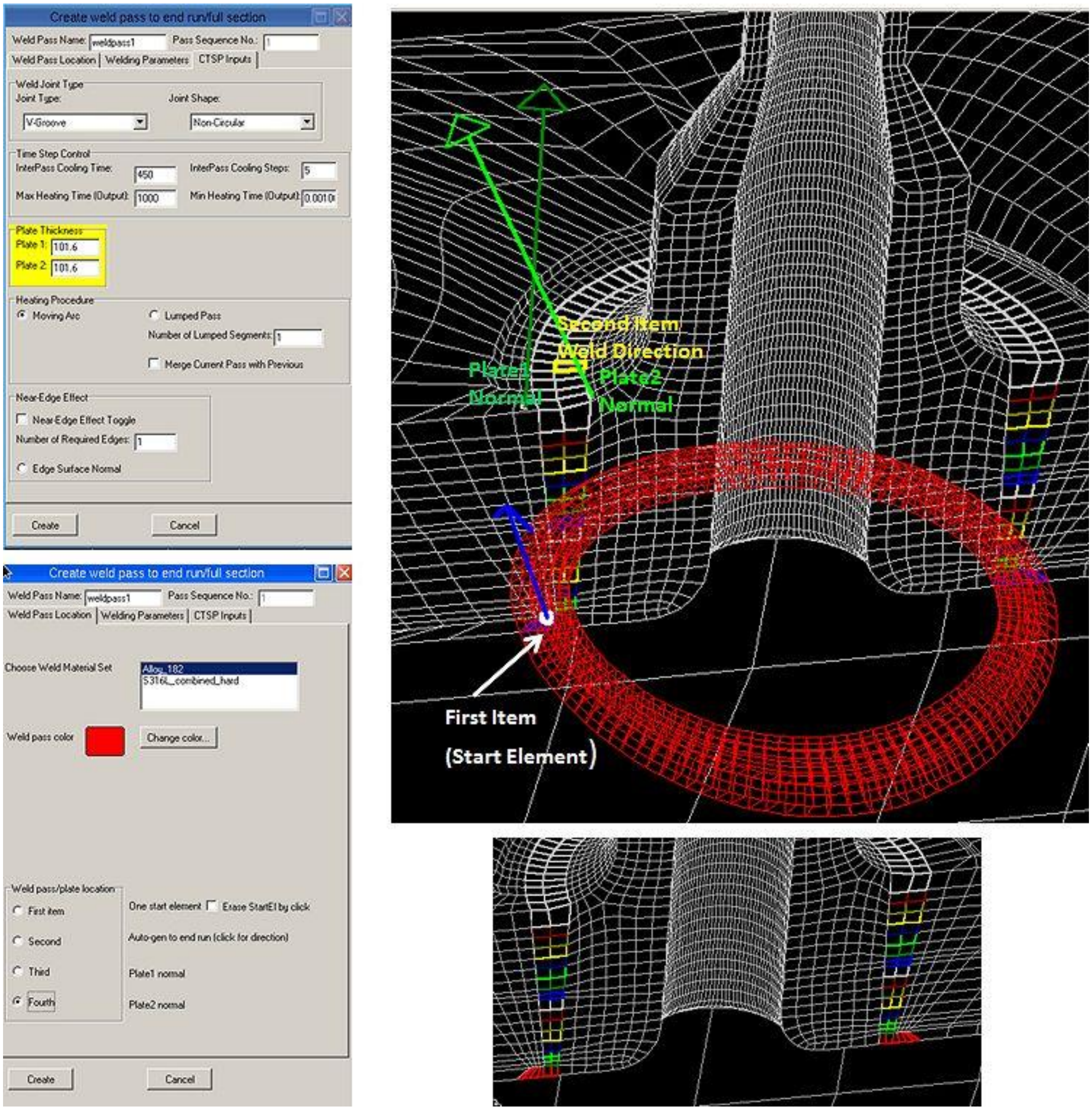


Figure 47 Creating weld passes

Step 4. Define boundary conditions. Here two nodes were fixed in all directions at both ends of the pipe (total of 4 nodes restrained) since this area is away from the weld and this mimics this pipe being part of a larger system.

Step 5. Write the CTSP and WARP3D input files. Here 16 cores were chosen for CTSP solution. Exit from VFT GUI and go to VFT App screen.

Step 6. Launch thermal solution. It took 8 minutes for the complete thermal solution, including merge and writing ParaView visualization files. This is many orders of magnitude faster compared to a numerical thermal solution (115,000 nodes here). Clicking on the 'Thermal' button permits us to view the weld fusion zone (Figure 48). ParaView is very powerful and intuitive to learn but the user should download the user manual. VFT is set up so that the desired visualization variables are invoked by clicking 'Apply' (red Arrow in Properties). The user can manipulate the view by rotation (left mouse click), Pan (press wheel down and move) or click one of the view axis (upper right Figure 48). The view in Figure 48 is a top view showing the fusion zone from the top looking down the nozzle. Also, the 'Clip' view can be invoked (upper left arrow Figure 48). By picking the correct cut view the user can see the cross section of the fusion zone. This view can be seen in Figure 49. The left and center illustration shows the maximum temperature experienced for all passes. This represents the fusion zone prediction with upper scale set to melting temperature of 1500 C. The right illustration provides the fusion zone for each individual pass (this is Pass 5).

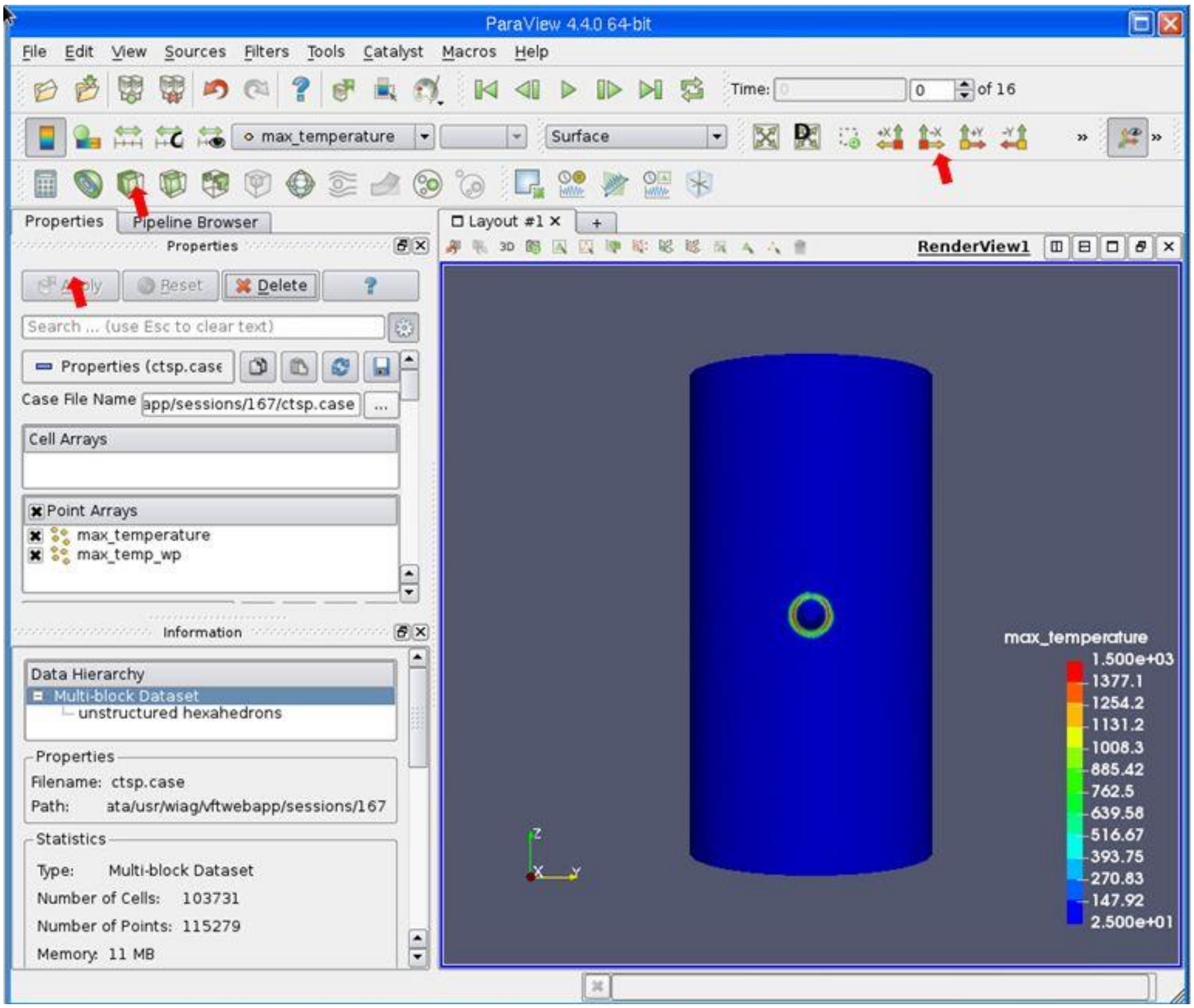


Figure 48 Click 'Thermal' button and invoke ParaView for fusion zone viewing

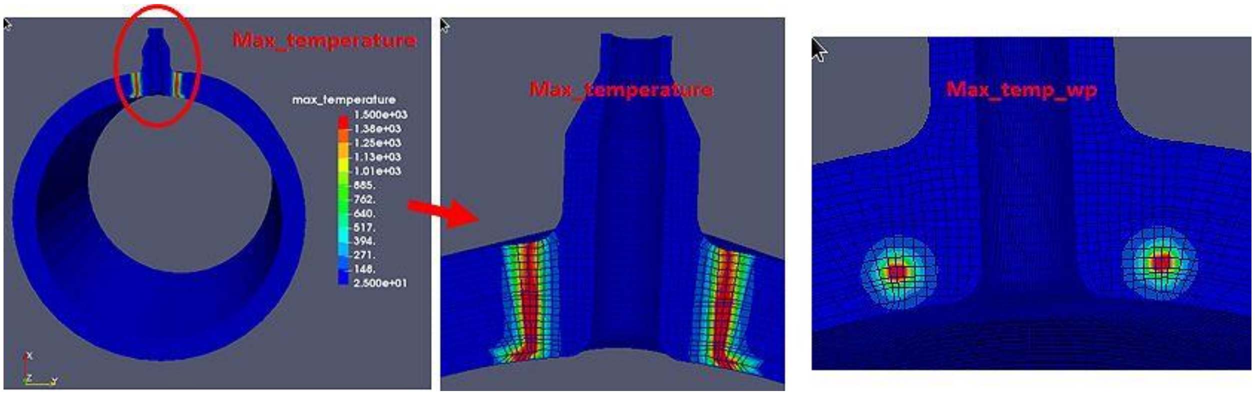


Figure 49 ParaView fusion zone visualization

Step 7. Click ‘Launch’ in Stage 3 to invoke the structural solution. For this case we chose to write out ‘Restart’ files and ‘Output’ results files every 100 steps (see screen in Figure 31 for lap problem). We also chose 10 hours for the estimate of solution time. Since there are more than 115,000 nodes this solution will take longer than 10 hours and we will restart. This is discussed in the next section where we review restart solutions.

Step 8. Examine results in ParaView. Click the ‘Structural’ button on Stage 4 (after WARP3D completes). This is illustrated in Figure 50. The user first clicks ‘Apply’, which is grayed out since we have already clicked it, to read in the values for viewing. These include stresses, distortions, plastic strains, temperatures, and other possible variables. At the top, click to the last time step (167 here – red arrow), perform a clip (upper left arrow), and the user visualizes the out of plane stresses. Note that the stresses to the left are slightly different from the right side since we started the weld passes at the left location.

Step 9. Redo analysis if necessary to achieve design goals or perform fatigue, fracture, or stress corrosion crack assessments as needed.

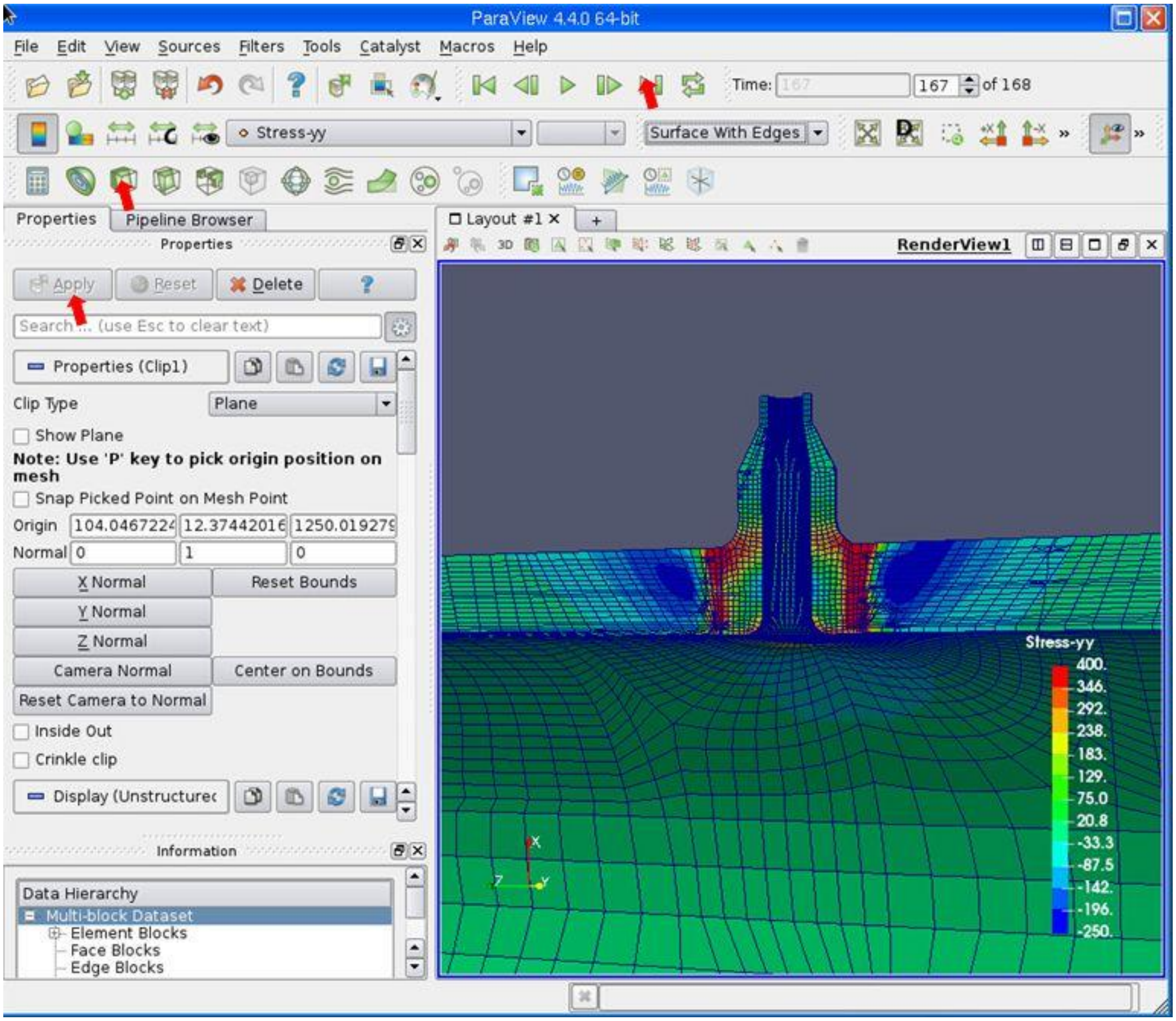


Figure 50 Out of Plane (Y) Stress

4.7 Restart Analysis

It is easy and convenient to perform a Restart analysis. This may be done for a number of reasons. The user may run out of allotted computer time. The solution may diverge and needs to restart with more increments (smaller time steps). The user may want to apply service loads overtop the weld residual stresses or distortions. We illustrate the restart analysis for the Head Nozzle problem since the user may have noticed that the 10 hours chosen for this problem were not enough to complete the analysis so the solution stopped.

4.7.1 Restart for Head Nozzle Tutorial Problem

For the head nozzle problem after running for 10 hours, which was the chosen solution time, the screen in Figure 51 appears. A message shows that it may have failed due to divergence. The user can click the 'Files' button and WinSCP takes the user to the file directory (red arrow Figure 51). Open the 'Results' directory. Open the 'logs' directory. The user can open the 'warp3d.log' to examine the WARP3D solution process. This will reveal whether divergence occurred or the user ran out of allotted computer time.

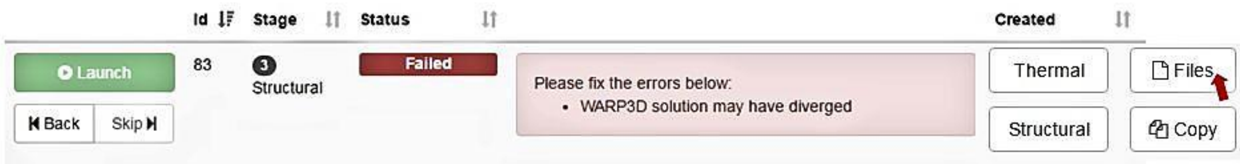


Figure 51 Failure screen for head nozzle problem after we ran out of time

To restart click 'Back' button (left side Figure 51). The user is sent to Stage 3 'Structural' again. Click 'Launch' and the Submit screen shown in Figure 31 appears. Here we show the full submit screen with parameters in Figure 52. The solution for the Head Nozzle problem was about 40% complete when we ran out of time (10 hours). Therefore we choose 15 hours for the restart solution. We again write restart information and output thermal profile steps as '100'. There is no need to change the solution step control parameters so we keep them at N1/N2/N3=1/2/2. Finally, the dialogue box at the bottom shows where we can pick which step to restart from. We choose the last step saved (700). Click 'Submit' button and the analysis will restart. This same procedure is used for divergence except then the N1/N2/N3 values need to be changed.

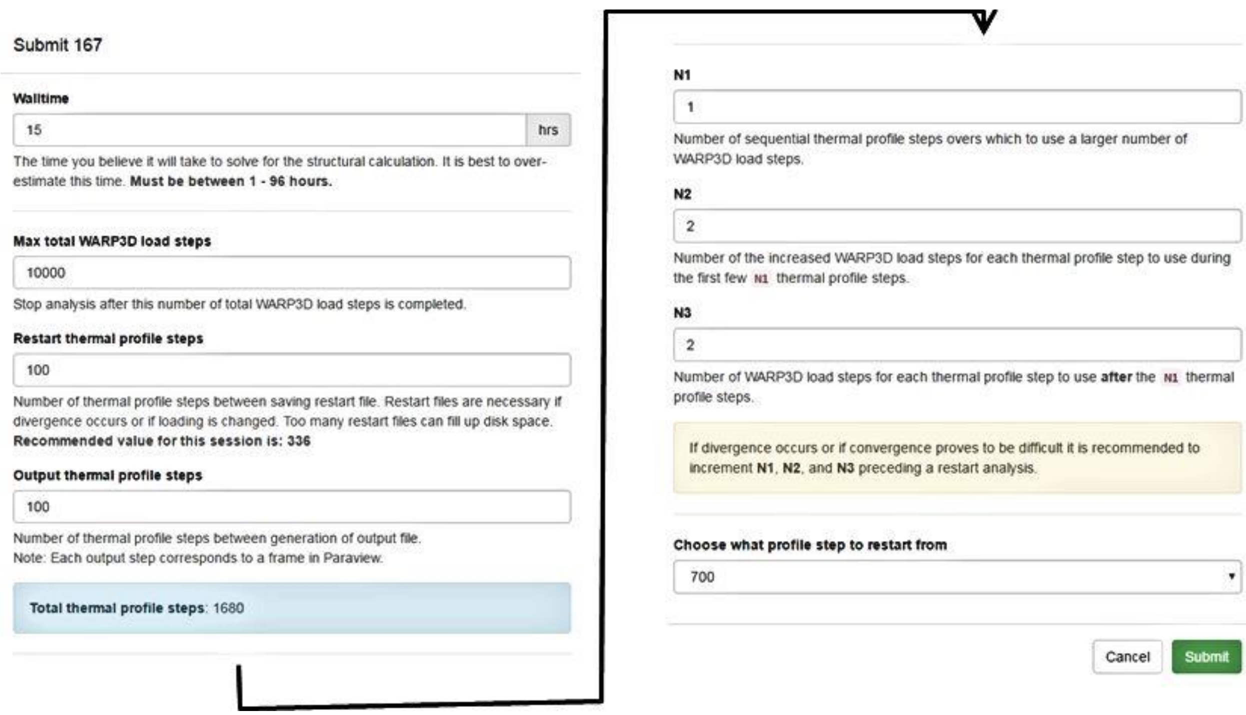


Figure 52 Submit screen dialogue box

5 VFT SYSTEM TECHNICAL DETAILS

This section provides details regarding the VFT modules that were improved in this DOE funded program. The three main modules, GUI, CTSP, and WARP3D were described in some detail in prior reports and References [1] and [2] and will not be repeated here. In addition, porting the system to the OSC system on AweSim is described as well.

5.1 The Graphical User Interface (GUI)

The weld GUI was written in C^{++} during this program and is invoked currently using a Windows system as described in Section 4. A number of user friendly and other necessary features for the non-weld modeling engineer were necessary and were implemented as discussed in both References [1] and [2] and in this section.

Preprocessing is the most labor-intensive aspect of simulation. Compared to larger firms, SMEs are relatively undercapitalized and understaffed, so the VFT® GUI preprocessor is a key element of successful adoption of the technology. The GUI was completely re-written in the latest version of C++ (Embarcadero C++ Builder XE7) to take advantage of new 64-bit programming features and is invoked currently using the Microsoft Windows operating system. Technically speaking, it also runs directly on the OSC Linux system by means of a WINE compatibility layer (www.winehq.org), but this needs further testing. HPC demands a diverse set of collaborative programming skills (e.g. graphics programming, system interfaces, MPI routines, etc.) so the entire VFT® code base is now resident on the industry-standard GitHub repository (git.com, with Microsoft Windows access by tortoisegit.org on AweSim OSC).

A number of user friendly and other necessary features for the non-weld modeling engineer have been implemented. Some of them are briefly discussed below and a more thorough description of other features are discussed in References [1], [2], and in Section 4 through the detailed tutorials.

5.1.1 Further GUI User Friendly Enhancements

Weld passes are specified by mouse-click on appropriate parts of the model. To enhance productivity, the GUI warns of imprecise clicks by immediate “Element not in a weld group” and “Element already in a weld pass” message boxes. Data on weld pass materials and normal directions, once entered for the first weld pass, are automatically applied to subsequent passes unless the user needs to change them. The tutorials discussed in Section 4 show detailed examples on the use of the VFT GUI and the training slides (Section 4.1). The GUI now writes multi-materials into WARP3D input files as well depending on the number of materials (up to ten materials) chosen by the user. This was coordinated into the WARP3D format for ‘user lists’, which is similar to the ABAQUS ‘*ELSET’ and ‘*NSET’ definitions. This facilitates easy implementation of multiple material problems. The menu items have been modified to be WARP3D specific and unnecessary buttons have been removed and more convenient buttons added. Many of the items shown in the Phase I report (Reference [2]) for the GUI have been streamlined in the re-write with Embarcadero C++ Builder XE7 and will not be detailed again here for the sake of brevity.

5.1.2 Material Library

Since VFT® is intended to be a “turnkey” solution for weld simulation by SMEs, it is essential that the complicated hardening nonlinear material properties of thermal elastic-plasticity be supplied as a simple library of material files. Figure 53 shows the pop-up menu for material file selection for weld passes, while Figure 54 shows the menu for non-WP parts of the model. There is a facility to enable users to attach their own proprietary materials file if desired.

The user clicks ‘Weld-Material Properties-Create’ and the menu on the right hand side of Figure 53 appears. If the user clicks ‘Browse’ they can then provide their own material file. Alternatively, the library of available material properties appears. An ‘iso’ in front of the name stands for isotropic hardening. ‘kin’ refers to kinematic hardening, either nonlinear or linear. ‘mix’ refers to Chaboche mixed hardening, while the simple and full ‘Leblond’ files refer to phase transformation plasticity laws. Descriptions of the file format for these are summarized in the UMAT manual. The file type should correspond to the user choice of constitutive law (isotropic, combined hardening linear, linear kinematic hardening, etc.).

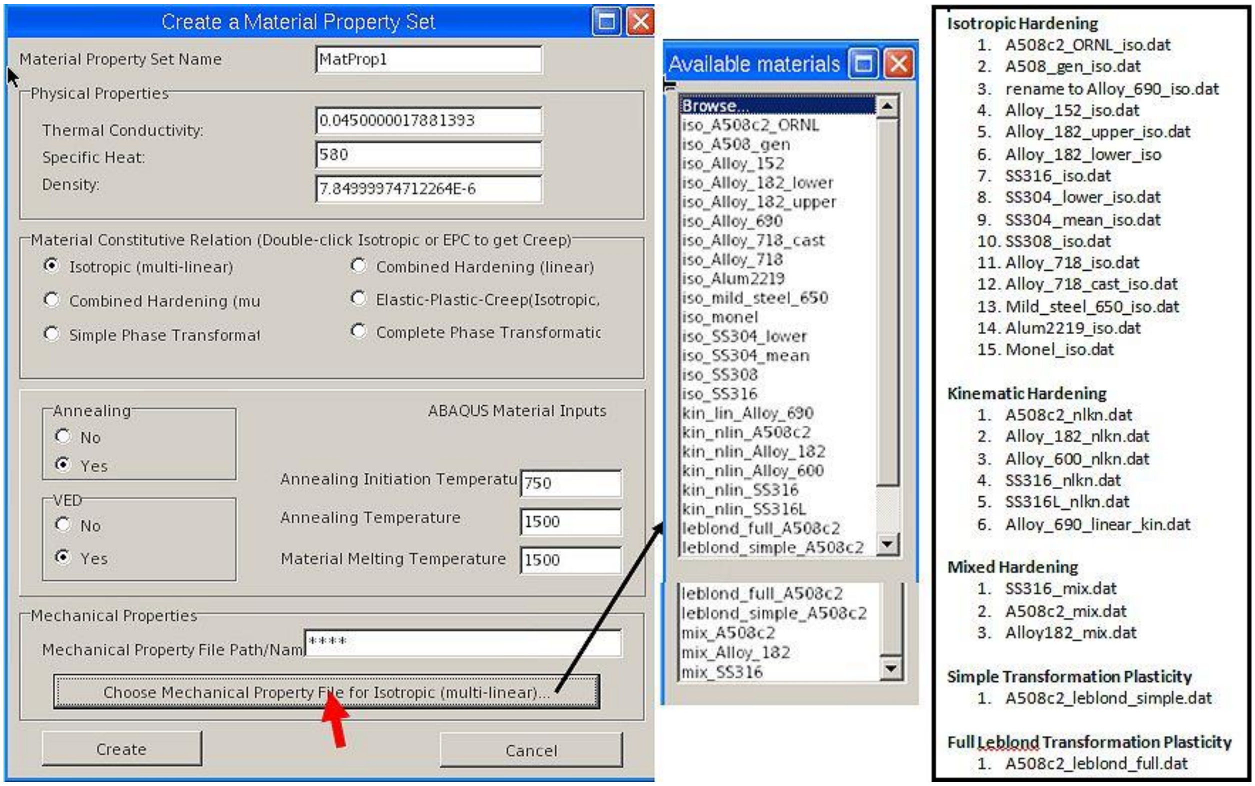


Figure 53 Material properties of weld metal, showing material selection from a list

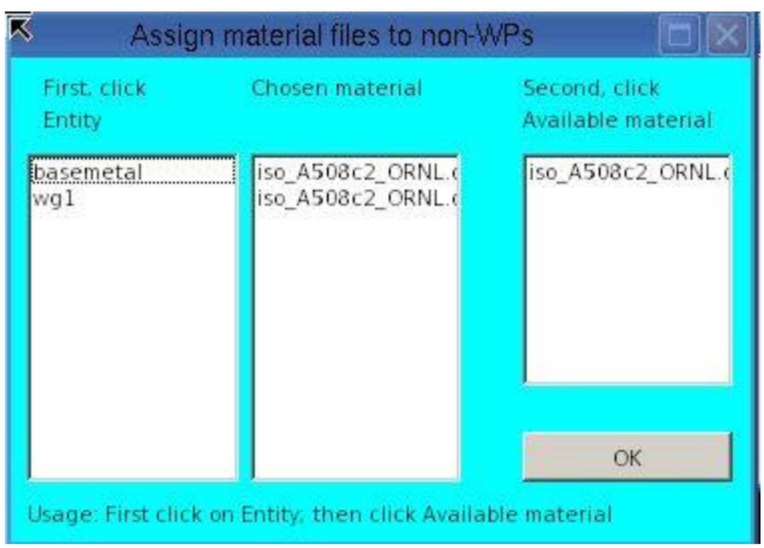


Figure 54 Dialog box to specify non-WP materials files from a list

Figure 54 shows the menu for picking the materials. This was already described with regard to the lap joint tutorial problem (Section 4.3, Figure 27). The material file names are descriptive. For example, A508c2 represents the vessel steel A508 class 2, Alloy_182 represents alloy 182 weld metal, SS 316 represents stainless steel type 316, and so on. More materials will be added as we obtain them. However, the user can provide their own materials as appropriate. In addition this will include choice of material for the various possible base metal groups that may exist in the fabrication to be welded. The data in the files include elastic properties and coefficient of thermal expansion versus temperature, uniaxial stress strain curves, nonlinear or linear kinematic hardening parameters, cyclic hardening parameters, and kinetic properties depending on the material law chosen. It is expected that many first time users of the system will choose isotropic hardening as this tends to produce upper bound residual stresses and distortions and the users will graduate to more complicated hardening laws as experience is gained.

5.1.3 Weld Specific Meshes

A library of example problems is available for download by the user from the documentation portion of the VFT App (See Section 3.2). The VFT® system requires hexahedral elements defined as extrusions along the welds where fine refinement is preferred. Many applications of welding involve relatively simple shapes, such as plates (or combinations of plates), cylinders, and spheres, for which elementary meshes are available. However, large complex geometries demand simulation and must be effectively meshed. These models are typically presented as IGES or STP files, which can now be meshed with hexagonal elements by commercial mesh generators.

Many SME users of VFT® will need to master weld control on simple geometries first. The user can also input their own mesh in a simple format for large problems which will require porting of files to the cluster. It is envisioned that a future enhancement to VFT will make this mesher general for large complex geometries. This is planned to be developed in the future. In the meantime, Emc^2 staff can help users develop meshes.

5.1.4 WRS and Distortion Visualization

The post processing of VFT® solutions within the WARP3D format requires the use of the DOE written HPC viewer called ParaView. The user defines the type of output and visualization desired within the GUI (for instance, distortions, stresses, etc.) Changes were implemented into WARP3D to permit writing out of solution dependent variables (SDVs) that are used within the UMAT routine depending on the material law that is chosen. At present there are 56 SDVs within the UMAT (see UMAT documentation available for download from the VFT App site. This permits post processing of all results to be made on the Portal via an app. See examples in Section 4. Since ParaView is Open Source the user can also download it to their desktop computer and view VFT results. This would require that the user port the VFT results files to their desktop after solution. The user can also download the latest User Manual from the ParaView site.

5.1.5 Testing and Validation

Extensive testing of the system was required prior to the trial launch on the VFT system on the AweSim platform at OSC. A number of weld problems have been solved on the system. These include the simple problems discussed in [1, 2] along with some new larger problems including the ‘plug’ problem shown in Figure 55 below [3] which also was detailed in a recent publication[§§]. During development and validation after each solution on the OSC system, results were compared to the same solution performed on the Emc^2 system with both WARP3D and ABAQUS to ensure solution accuracy and solution speed is maintained. Upwards of 50 examples were verified in this fashion. It is important to note that the OSC

[§§] Other example problems are available for download in the Publications download portion of the VFT App.

system has faster computational solution times compared to the Emc^2 system (for the same number of processors used) and WARP3D solutions are faster compared with ABAQUS for these same problems. These problems are not detailed here as the user is referred to Section 8 of [2] for some of the problems being solved. Many of the problems discussed in References [4,5] using ABAQUS were also solved on the VFT OSC system for validation. Validation with measured data can be found in the publication download portion of the App. These are for thermal validation with thermocouple data, distortion validation with laser sensors, and residual stress prediction validation via measurements. In the documentation section are lists of publications that may be relevant for the VFT user. These are compiled under four different categories: crack growth modeling, VFT theory, WRS papers, and VFT validation.

This testing ensured that the system is stable, easy to use, and accurate. This ease of use and user friendly nature of the system was assessed through use of an inexperienced weld modeler recruited from welding engineering students at The Ohio State University here at Emc^2.[***]. In addition other organizations also tested out the system on problems of direct interest to their organizations during training and through the system tutorials. After the initial testing, the trial users of VFT® were given access for further enhancements of the user friendly nature of the code. This activity will continue forever.

5.1.6 Subcritical Crack Growth Analysis

Another long term vision for VFT® on the AweSim OSC Portal is to permit the user to perform subcritical crack growth and life assessments using the system. Weld residual stresses have been found in recent years to play a pivotal role in life predictions where they were often ignored in the past. Both fatigue and stress corrosion life assessments are anticipated to be made available with the system in a future release. Fracture in weld residual stress fields is not important except in brittle materials since the weld strains at the crack tip are 'washed' out by the plasticity at the crack tip in general. The current plan is to tie a finite element alternating method (FEAM) fracture code[†††] for evaluation of stress intensity factors for these growth assessments. Currently fatigue crack growth is performed after the weld modeling in a separate analysis. In addition, in future planned work, 'natural crack growth' will be tied to PipeFracCAE© (another Emc^2 software tool) for odd shaped cracks often caused by stress corrosion crack growth (crack growth publications list in documents section).

5.2 Thermal (CTSP) Solution Enhancements within the Portal System and Temperature Visualization

The speed, validity and accuracy of the CTSP system were discussed in Section 7 of the DOE Phase I final report [2]. Here a brief summary of the improvements made to the code are summarized.

5.2.1 GUI/CTSP Improvements

The CTSP rapid thermal solver was improved to permit multiple core solutions and merge of the results into a thermal file. The current procedure for performing the thermal analyses within the framework of the enhanced VFT code is discussed by reference to an example problem that was solved using the system on the OSC portal. Figure 55 illustrates a plug weld example that might represent a repair weld in a nuclear pressure vessel. An Alloy 690 plug is to be welded to a stainless steel clad head using Alloy 52/152 weld metal. This is an illustrative problem of the type that may occur in the field. Figure 56 shows the VFT GUI view of this plug weld. Details of this recent practical example are provided in [3].

[***] Dr. Brust is a guest lecturer to the department for computational weld modeling.

[†††] This code is owned and leased separately by Emc^2 and can be ported to the Portal.

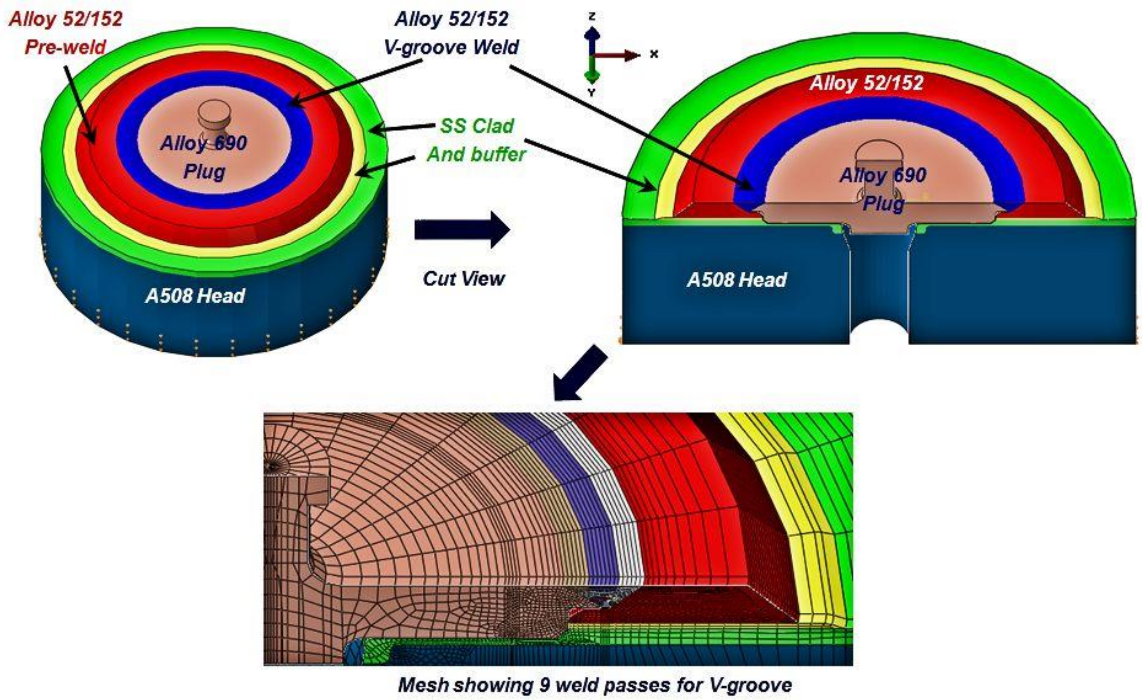


Figure 55 Plug weld example (sanitized proprietary example)

The steps in developing the model consist of the following for the CTSP thermal solution.

1. Read the model into the GUI.
2. Define the material properties.
3. Define the weld passes. For this example there are 9 passes.
4. Define boundary conditions. These consisted of constraining the vessel head at the boundaries (see [3]).
5. Export CTSP files (File-Export-CTSP).
6. CTSP solutions are then performed in each subdirectory on different cores. This produces ASCII text files in each subdirectory (temp.out). The different temperature files are then merged using a FORTRAN utility. This merge procedure routine is quite involved since the overlap of a solution performed on one core must properly combine with that produced on each other core. A 'cutoff.exe' FORTRAN code is then executed to ensure temperatures predicted by CTSP are not above melting. This is possible since CTSP (see [1]) is a series solution of a core closed form solution and if a node is too close to a heat source the temperature can become artificially higher than melting. However, this does not affect the subsequent WARP3D solution. Finally, the ASCII temperature file is converted into a binary file with a corresponding text file which is used by WARP3D to optimize the solution process. This is a FORTRAN utility called 'TEMP_CONVERT'.
7. Perform the WARP3D analysis by clicking on the 'Launch Structural' button in Figure 9 bottom illustration
8. Examine results in ParaView.
9. In this case a number of plug designs were considered along with repair welds. The design was optimized via a number of analyses (more than 40 total). See [3] for details.

This design was then successfully implemented remotely in the field in a European reactor.

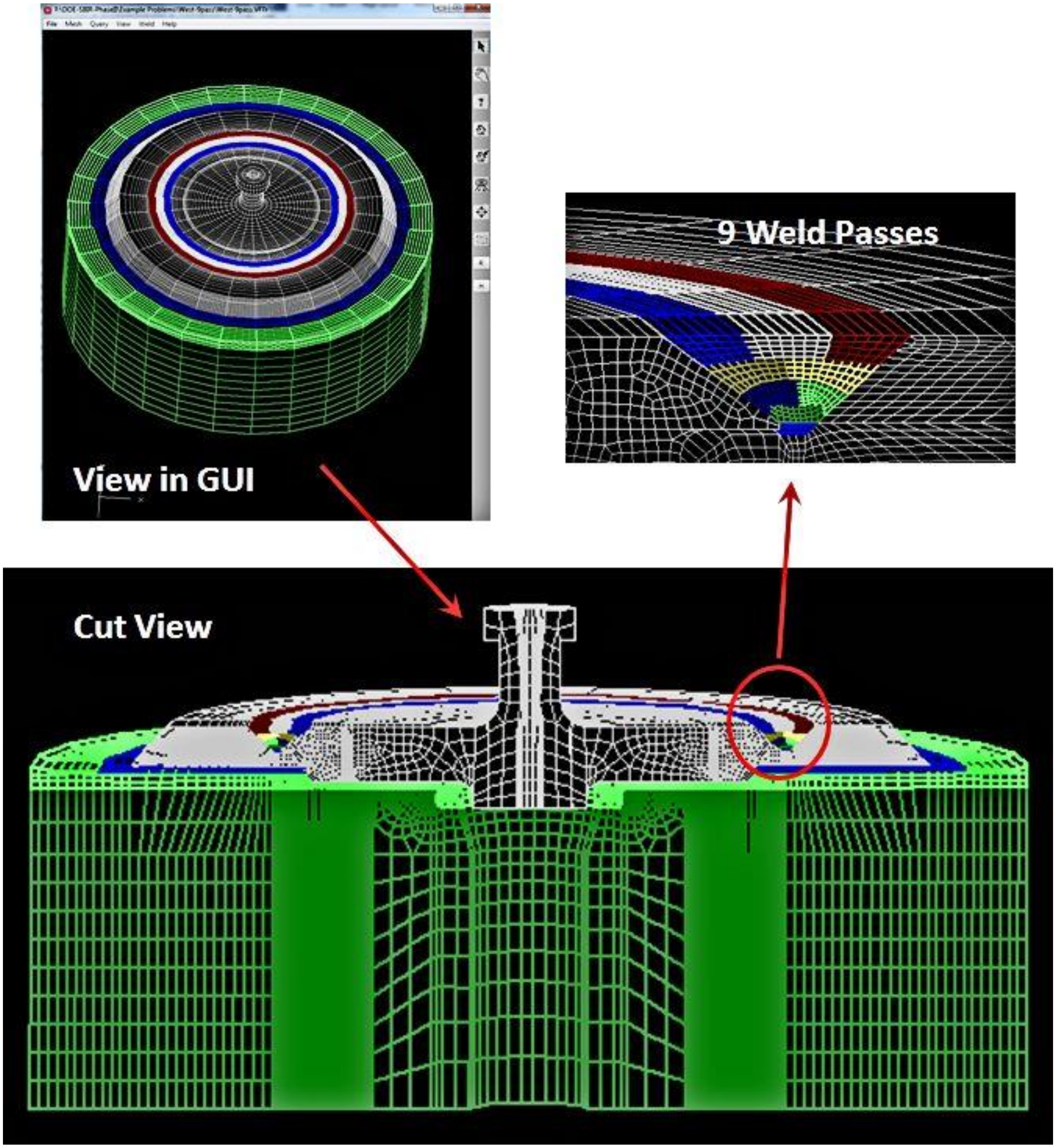


Figure 56 VFT GUI view of plug weld

After the user defines all materials and weld passes and is ready to write out the files necessary for performing the VFT analysis, the following dialogue box shown in Figure 57 appears. The desired file name is requested and the number of cores for CTSP solution is requested. The core loads are automatically balanced in writing out the CTSP input files. For this problem, with 9 passes, 4 cores were used. This automatically creates 4 subdirectories (CTSPsubd001 through CTSPsubd004) with the necessary input files for performing CTSP analysis.

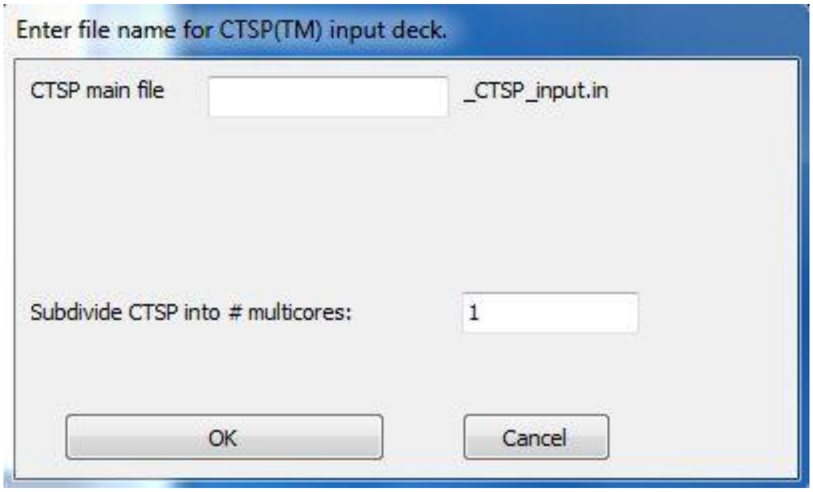


Figure 57 CTSP export command within the GUI

5.2.2 Thermal Profile Concept

An important advance made to the thermal/WARP3D solution process is related to Step 6 above. A summary of the new procedure used to ensure convergence of the WARP3D solution is provided. Recall that originally WARP3D was not made to solve the weld problem, and in fact WARP3D does not even have a thermal solver. This is not necessary for the casual user but the advanced user may want to study this section.

- The thermal and stress analyses are de-coupled. This has been shown to be adequate for computational weld analyses.
- Post-processing of the thermal analysis produces 2 files for WARP3D-VFT simulations to define thermal profiles as seen in Step 6 above.
- A thermal profile is a list of updated (total) nodal temperatures at time t_i during the weld simulation.
- Profile 0 is at time $t = 0$. All model nodes have the reference temperature defined in WARP3D input file. No temperatures needed from profile definition. If pre-heat is defined prior to the weld analysis then the pre-heat temperature is defined within the GUI as the initial temperature.
- WARP3D linearly interpolates nodal temperatures when required for simulation times between profiles. This is further discussed in [1] and [2]. This interpolation feature was recently added.
- WARP3D simulations always begin and end on specified profile times – no WARP3D load (time) step spans into the next profile.
- A WARP3D simulation from profile i to $i + 1$ uses n load (time) steps. n is sometimes equal to one.
- Profiles are defined via 2 files: <name>.txt and <name>.bin. These are produced by the TEMP_CONVERT.exe routine described in Step 6. <name> is arbitrary – often chosen to describe model.
- Contents and format of <name>.txt are defined. File may have comment lines for documentation. These are defined automatically for the user.

- <name>.bin is a binary “stream” file. Consists of pairs: <node #> <temperature> <node #> <temperature> ….. These are produced by applying Step 6 to the temp.out file produced by CTSP.
- <node #> is 4 bytes, <temperature> is 4 bytes (float)
- Temperatures are absolute; WARP3D subtracts reference value from all specified profile values at analysis start.
- Those nodal temperatures specified for a profile ***replace*** prior temperature values for nodes (usually only a fraction of the model nodes have updated temperature values specified in a profile)

The <name>.txt file is a concept for prescribing nonlinear solution procedures within WARP3D for computational weld problems within VFT. The format is illustrated in Figure 58. It is critical that divergence rarely occurs for VFT on the Portal since users are not expected to be experts with nonlinear finite element analysis. An automatic ‘restart’ capability will be added in case the rare event of a divergent solution occurs. This new concept has not resulted in divergence in any test problems performed to date.

Referring to Figure 58, the following summary of the parameters is defined. Information about each thermal profile necessary for TEMP_CONVERT to produce this file is defined in the param.in file which is written out by the GUI based on knowledge about the weld passes. The comments within the uexternal file (Figure 58) describe these definitions. Again, only the advanced user should want to know this. More details are also discussed in Section 5.3.2 regarding the step size definitions (N1/N2/N3). By default the GUI writes these out as N1/N2/N3 = 1/2/2. However for some problems the user may want to change these (See also the ‘Submit’ screen definition in Figure 52).

```
! Three non-comment lines with file names required
!  1 - name of material.dat file for VFT
!  2 - name of VED.dat file
!  3 - root of file names for thermal profiles
!      There must be file names with extensions
!      *.txt & *.bin
!      Omit extensions here.
!
! File names may have ~/ to denote user home directory.
! WARP3D will resolve to full path name.
! NEXT Line is the number of materials (up to 10),
! Followed by material files (here A508c2.dat)
!VED.dat file
! and thermal files (stay the same)
1
./A508c2.dat
./VED.dat
./warp_temp_2_files
!
! Stop when analysis for this thermal profile completed.
! If this number of profiles is not defined, WARP3D will
! write output files, a restart file, and execute normal termination.
!
 10000
!
! Values to control output:
! - number of thermal profiles between saving restart file
! - number of thermal profiles between generation of output file
! - file of WARP3D output commands to be executed
!
 30, 10
output_commands.inp
!
! Values to control solution when:
! o - a torch or torches comes on
! o - cooling starts
! o - analysis startup and on restarts
!
! - (N1) number of sequential thermal profiles over which
!       to use a larger number of WARP3D load steps
! - (N2) number of increased load steps to use (>=1) for
!       solution over these profiles
!
 1, 2
! Value to control solution when:
! o - heating is occurring and has continued beyond N1 above
! o - cooling is occurring and has continued beyond N1 above
! - (N1) number of sequential thermal profiles over which
!N3 is the number of load steps per profile for all profiles after the number of
!profiles dictated by N1.
!
!For example,  N1 = 5, N2 = 10, N3=15
!The first 5 profiles in any heating or cooling cycle will use 10 load steps per profile.
!All load steps after that in that profile will use 15 load steps per profile. Then it
!starts again at the next heating or cooling cycle.
!
! N3 =1 is the most common value.
!
 2
```

Figure 58 Format for the 'uexternal_data_file.inp' used to control WARP3D solution

The introduction of this information has made the corresponding WARP3D solution very stable and has improved solution speed for the thermal plasticity based computational weld problem. Prior to the introduction of this solution, control file computational weld analysis problems using WARP3D were somewhat unstable. The VFT user has no need to understand the details of these algorithms as this is automatically produced by the GUI and corresponding utility routines.

5.2.3 – Thermal Solution and Viewer

After the thermal solution is complete, but prior to the structural solution, the user should interrogate the temperature fields. This usually means checking the weld fusion zone to ensure that proper weld parameters were defined to ensure a reasonable solution. This will invoke ParaView where the results on cross sections can be made. The routines discussed for transferring the temperatures into a binary file, prior to conversion into a format useful to ParaView, are being modified.

The process of developing necessary files to perform the CTSP-based thermal analysis for VFT weld solutions currently requires a number of routines. These are illustrated in Figure 59.

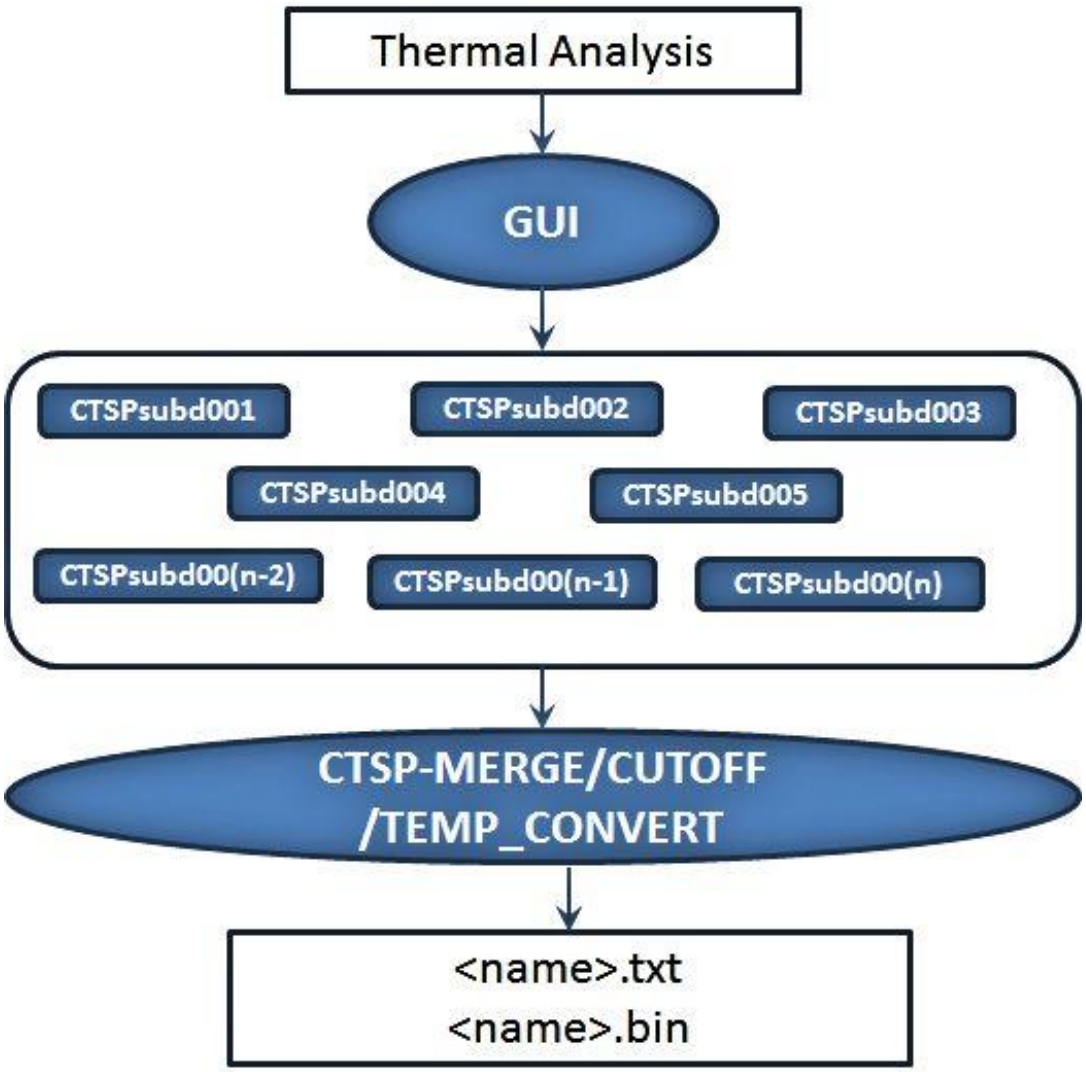


Figure 59 CTSP thermal solution procedure

In Figure 59 the GUI is used to write out a series of CTSP subdirectories. These range from 1 to n, where n is the total number of processors to be used to produce the thermal solution. At present the user chooses the number of processors to use based on problem size, number of welds, etc. This algorithm was written to automatically 'load balance' the cores so that each will require roughly the same solution time. Next, the CTSP-MERGE routine merges the individual temperature files created on each core by calling each individual directory (or core) and combining the results into a large ASCII file. Next the CUTOFF routine is used to ensure the maximum temperature is melting and finally TEMP_CONVERT creates a binary temperature file (which is read very rapidly within WARP3D – called <name>.bin – and produces <name>.txt which manages the thermal solution procedure within WARP3D so that the it knows when weld torches are arriving, stopping, etc., leading to stable solutions. This is automated and transparent to the user.

5.3 Stability of Open Source WARP3D Weld Specific Analysis and Addition of Weld Specific Features

The speed and validity of the VFT® system as tied to WARP3D were discussed in Section 8 of the DOE Phase I final report and Phase II interim report [1, 2] as were the improvements needed. VFT® was originally tied to the general purpose commercial code ABAQUS prior to the Phase I program. ABAQUS has some useful features that are necessary to make VFT® more useful for general purpose applications. In addition, a critical feature of VFT® residing on the OSC Portal for use by general users is that the system must be stable. This required some additional features to be added to WARP3D to ensure solutions converge always[‡‡‡]. These are briefly discussed below and more details can be found in [1, 2].

5.3.1 Solution Speed, Stability and Restart Enhancements

A number of enhancements were made to permit forward time stepping algorithms and other features necessary to improve solution speeds with WARP3D for weld problems. The VFT solution process with WARP3D has been streamlined and refined as summarized in the following topics.

Simpler user input to define model & nonlinear solution procedures

Some of the convenient new features added to the VFT/WARP3D include:

- Much simpler user input to define model & nonlinear solution procedures
- Large number of thermal profiles consolidated into a small ASCII text file and a corresponding single binary file
- Small input file for *uexternaldb* routine to provide guidance on solution procedure and file names
- Nonlinear analysis now focuses on advancing solution from thermal profile i to $i + 1$ rather than load (time) steps
- The *user_solution_parameters* routine drives computations from profile i to $i + 1$ automatically using WARP3D load (time) steps
- Simplified control of output file generation & writing restart files at completion of a profile
- WARP3D nonlinear steps/iterations more stable
- Analysis checkpoint and restart, if needed, fully supported

For a VFT simulation the WARP3D finite element model must contain: VFT weld specific user routine (UMAT) (weld specific material laws depending on the material law chosen), element type(s) and

[‡‡‡] It is noted that VFT® is completely stable when using ABAQUS.

properties, nodal coordinates, element connectivity (*i.e.* "incidences"), displacement constraints on nodes, initial nodal temperatures at time 0, thermal loading (new reference to *user_nodal* routine), mechanical loadings if any, nonlinear solution parameters, a (text) file of compute commands (the same file is used in all WARP3D-VFT analyses), thermal profiles, material.dat file, a VED (virtual element detection) file which is used within the UMAT to permit weld elements to be activated at the proper time when the weld torch arrives, and a *uexternal_data_file.inp* which defines material.dat and VED.dat file names, root file names for thermal profiles, file name for WARP3D output commands, and restart file information. VFT uses a 'progressive annealing' features to account for material history loss at very high temperature [6].

The current format for the VFT based WARP3D input file is shown in Figure 60 and Figure 61 with the corresponding line numbers for the submarine tutorial problem discussed in Section 4.5. This file is automatically written out in its entirety by the GUI. It is anticipated that some users of VFT on the AweSim OSC system may use the system entirely as a 'black box' without knowledge of the actual input files. However, as users become more advanced they may want access to the files so that changes and modifications can be made directly. The compact nature of the entire input file shown in Figure 60 and Figure 61 is quite convenient. The User Manual and the Wiki on the Portal will specify these but a short description is provided below with reference to Figure 60 and Figure 61.

- structure name – line 1 (structure sub) – use any name during definition with the GUI
- vft-umat name and global properties definition (line 5 and 6 to 10). This UMAT is not available to the user unless agreed upon
- mesh counts (nodes and elements) – line 16
- list of element group definitions (weld passes, plates, other definitions). This is stored in the file 'sub.list' seen in Figure 42 –line 18
- nodal coordinates input file – line 19 'sub.coordinates' Figure 42
- element definition & properties – lines 22 to 31. Here we use by default for VFT problems the 8-node linear displacement element (I3disop). This has a B-bar formulation to prevent volume locking. We specify a linear small strain formulation (which for most weld problems is adequate but this can be changed by the user). A 2 x 2 x 2 Gauss integration order is standard for weld analyses. In addition line 27 specifies stress-strain output averaged at element center ('center output'), and 'short' output option omits principal values and directions. For the submarine problem there are 4 element groups (in sub.list) defined: basemetal, and passes WP1 to WP3.
- incidences (element connectivity) input file – line 33
- blocking assignments (now done automatically for VFT/WARP3D) – line 35
- displacement constraints file – line 38
- initial (reference) temperatures for nodes – lines 40 to 44
- patran neutral file definition (for use with ParaView visualization) – line 46
- one loading condition (termed "pattern" in WARP3D) - *user_routine* option causes thermal profiles to be processed – lines 52 to 54
- single nonlinear loading condition to set steps and nonlinear loading name *must be weld_sim* – lines 59, 60
- Just define 10000 steps so we have more than needed. May need more for huge problems in the future – line 61

```
structure sub
c
c
c
c Material VFT UMAT commands
material A508c2_umat
  properties umat  rho 0.0  alpha 0.0,
       um_1 1 um_2 750 um_3 1500,
       um_4 1500 um_5 -1.0,
       um_6 -1.0 um_7 0 um_8 0
c     ***************************************
c     *          end of materials           *
c     ***************************************
c
c
number of nodes 16080 elements 12548
c
*input from 'sub.list'
*input from 'sub.coordinates'
c
c
elements
c   for config number   0
"basemetal" type l3disop material A508c2_umat order,
 2x2x2 center_output short
"WP1" type l3disop material A508c2_umat order,
 2x2x2 center_output short
"WP2" type l3disop material A508c2_umat order,
 2x2x2 center_output short
"WP3" type l3disop material A508c2_umat order,
 2x2x2 center_output short
c
*input from 'sub.incid'
c default blocking is 128 elem/blk
blocking automatic
c
c
*input from 'sub.constraints'
c
c  Define initial temperatures
initial conditions
   temperature
         nodes 1-16080 temperature 25
c
output model flat patran convention text,
  file "sub_flat"
c
c  From the template here are the load definitions.
c  Total weld times are also included for convenience, not necessity
c
*echo off
```

Figure 60 Example VFT/WARP3D input file for Submarine problem (lines 1 to 49)

```
52 loading weld_temps
53  nodal loads
54   user_routine
55 c
56 c The loading steps
57 c
58 c This name must be used in the following: weld_sim
59 loading weld_sim
60  nonlinear
61   step 1-10000 weld_temps 1.0
62 c Always define 5000 or more steps
63 c Actual number of steps solved is determined dynamically by the
64 c user_solution routine in response to features of thermal profiles.
65 c
66 c
67 c Solution parameters.
68 c
69  nonlinear analysis parameters
70  user_routine on
71  umat serial off
72  solution technique direct sparse
73  convergence test maximum residual tolerance 0.5
74  nonconvergent solutions stop
75  divergence check on
76  batch messages on
77  cpu time limit off
78  material messages off
79  bbar stabilization factor 0.05
80 c The following is only used for large displ analysis
81  consistent q-matrix off
82  trace solution on
83 c The following values ignored because controlled by user_routine
84    time step 0.09436531
85    maximum iterations 7
86    minimum iterations 1
87    adaptive solution on
88    linear stiffness for iteration one off
89    extrapolate off
90 *input 'compute_commands_all_profiles.inp'
91 stop
92
```

Figure 61 Example VFT/WARP3D input file for Submarine problem (lines 50 to 86)

- Solution control parameters optimized with WARP3D for VFT weld problems – lines 69 to 89. See the WARP3D manual for definitions.
- ‘compute_commands_all_profiles.inp – line 90. This file can be observed by opening it (Figure 42)

The nonlinear solution parameters (lines 69 to 89) have been optimized for weld. These values have been recommended based on current experience with VFT analyses. The values in Figure 60 and Figure 61 are currently recommended values and are automatically printed out by the GUI. The order of options is not important.

- user_routine on (must use UMAT for weld problems) – line 70
- umat serial off (specify UMAT optimization for use with multiple cores) – line 71
- solution technique direct sparse (use of iterative solver for weld problems needs further work) – line 72
- convergence tolerance may need to be reduced for analyses to compute residual stresses – line 73
- *bbar* value can be reduced to zero or 0.01 if possible. We currently set to .05 – line 79.
- large displacement analyses – not necessary for weld problems
- line 90 reads in all compute commands from a file. The format for this file is illustrated in Figure 62. This same *compute_com…* file may be used for all VFT WARP3D analyses (except restarts). <u>*Note*</u>: name of loading is *weld_sim* as defined in line 59. The file *vft_solution_cmds.inp* is created by the *user_solution* routine – on the fly – during the solution. Users do not create or modify this file. This routine contains various *output*, *restart*, and eventually *stop* commands. For restart analyses this file is automatically changed appropriately.

It is emphasized that for SME use of VFT on the OSC all of these files are automatically produced by the GUI and the user does not need to know these procedures. However, it is useful for advanced users to know the mechanics of the VFT/WARP3D system.

```
!
 compute displacements loading weld_sim step  1
   *input from 'vft_solution_cmds.inp'

 compute displacements loading weld_sim step  2
   *input from 'vft_solution_cmds.inp'

 compute displacements loading weld_sim step  3
   *input from 'vft_solution_cmds.inp'

 compute displacements loading weld_sim step  4
   *input from 'vft_solution_cmds.inp'
         .
         .
         .
compute displacements loading weld_sim step  9999
   *input from 'vft_solution_cmds.inp'

 compute displacements loading weld_sim step  10000
   *input from 'vft_solution_cmds.inp'
!
stop
```

Figure 62 Format for *compute_commands_all_profiles.inp*

5.3.2 Enhanced Solution Strategy for VFT/WARP3D

As alluded to above a number of features have been added to VFT so that solution with WARP3D is stable. The goal is to ensure that all computational weld problems run with WARP3D have a very unlikely possibility of diverging. For an SME performing a VFT weld analysis on the OSC Portal, solution divergence must be avoided. However, in the event that divergence does occur, procedures have been developed within the GUI to permit seamless restart of a divergent solution to ensure analysis completion. This section provides some more details of the uexternal_data_file.inp first discussed with regard to Figure 58.

With reference to Figure 63, values N1, N2, N3 are specified in text file: *uexternal_data_file.inp*. WARP3D *automatically* drives the welding simulation from profile *i* to *i* + 1. One or more WARP3D load (time) steps is used to discretize nonlinear response from profile *i* to *i* + 1. Nodal temperatures vary linearly between profiles. The user specifies last thermal profile for simulation. This is all automatically driven by the GUI so the user does not need to know these details.

The user controls algorithm through three input values:

N1: when a heating/cooling period begins, the number of consecutive thermal profiles over which WARP3D *will* use a larger number of load (time) steps

N2: number of uniform load (time) steps to be used over each profile in N1 region

N3: number of uniform load (time) steps to solve each profile during steady heating/cooling (often = 1)

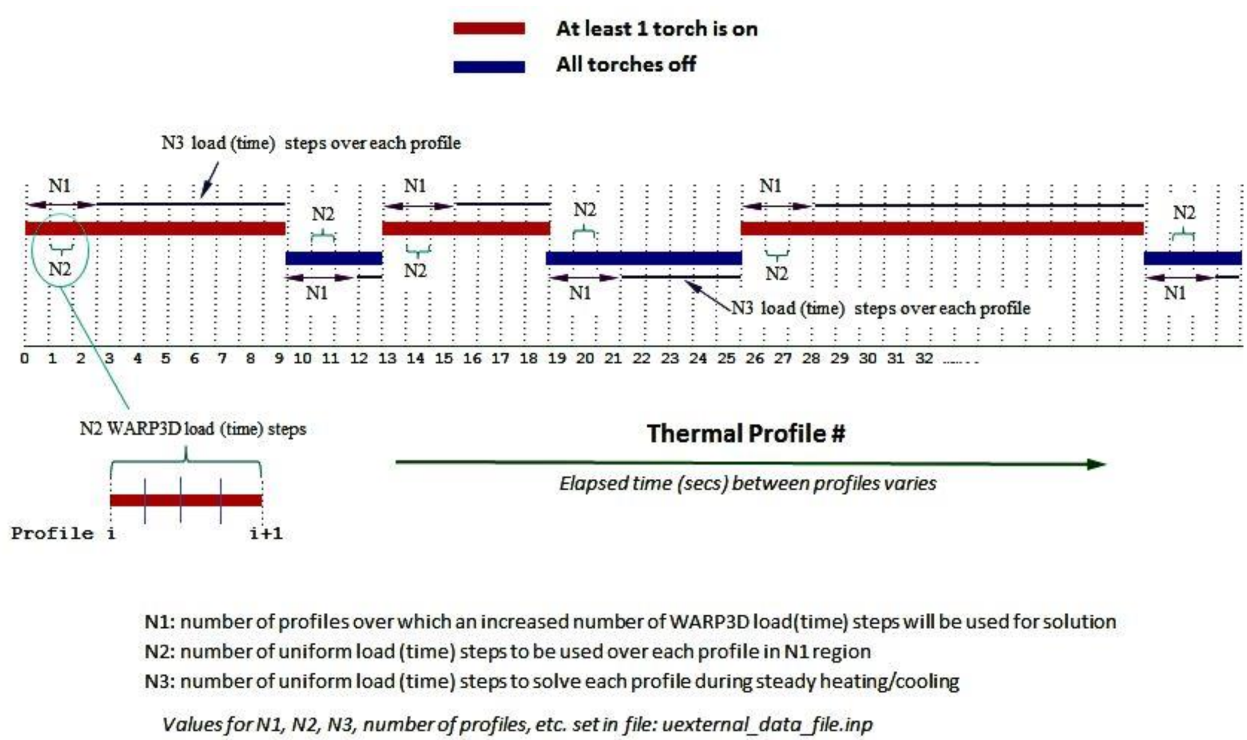


Figure 63 Enhanced solution strategy based on concept of automatic controls

In the *uexternal_data_file.inp* file, the user also specifies:

- Frequency of thermal profiles between writing of checkpoint/restart (.db) files. For example, value of 5 causes restart file writing after profiles 5, 10, 15, 20, … are completed
- Frequency of thermal profiles between writing of output data (printed output, Patran compatible result files, etc.)
- Name of a text file that contains WARP3D *output* commands to be executed (usually just *output_commands.inp*)

The VFT UMAT code, which is a weld specific user routine (discussed in Reference [2]) has a number of weld specific material laws for the user to choose. Because it is a user routine, and there are numerous material laws to choose from, there are a number of constitutive law internal variables (solution dependent variables, or SDV's in ABAQUS) that the user may have interest in viewing. For instance, if the user chooses a phase transformation plasticity material law, it is of interest to observe the material phases that are predicted.

5.3.3 Example Profile/Load Step Study

A number of studies have been performed in an effort to optimize the N1, N2, and N3 automatic time stepping procedure discussed above. Presented below is an example of the 966H pant leg model which was extensively studied in the Phase I program (see Reference [2]). This problem has 51,781 nodes, 41,598 elements, and 36 weld passes. The N1/N2/N3 values used are shown in all four cases (additional cases were considered without good performance) in Figure 64. The upper left case (N1/N2/N3=1/2/2) produced the fastest runtime of 3 hours 5 minutes with no convergence problems. As seen in Figure 64, the other cases using different values of N1/N2/N3 did not perform as well. Moreover, it appears that N3>1 appears to be critical to convergence. Other examples were run as well and the N1/N2/N3 sequence of 1/2/2 appears to be optimum for ensuring convergence and good run times

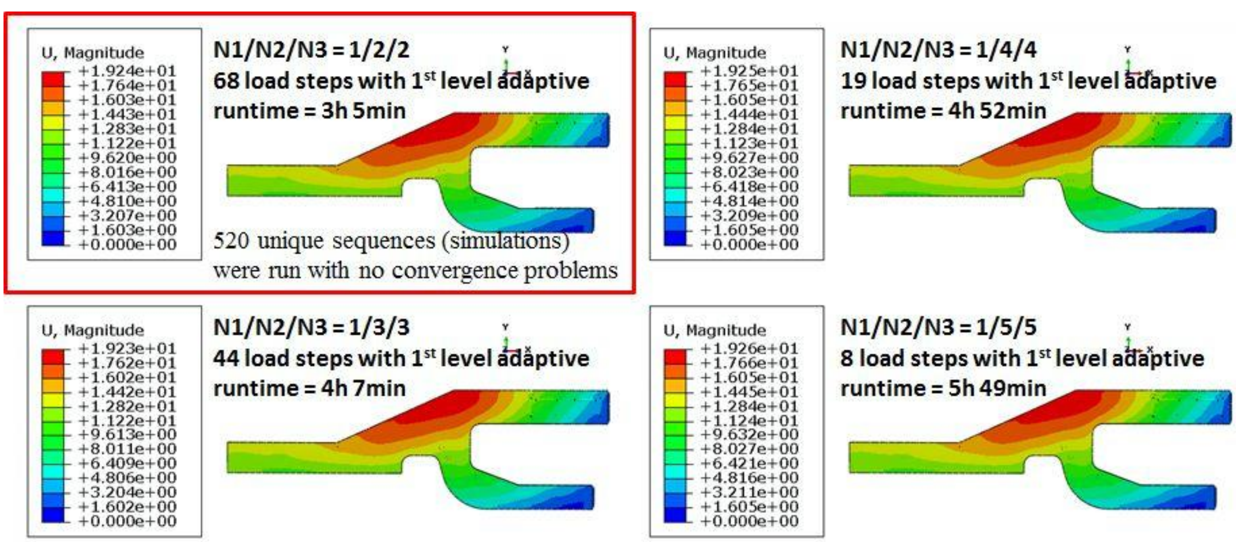


Figure 64 Pant leg problem used for solution parameter optimization

In addition, some other improvements have been made that are briefly discussed below.

- Restart capabilities for VFT/WARP3D have been developed and analyses have been performed showing that the procedures work.
- Boundary constraint changes are possible also. For instance, a distortion control strategy, called pre-cambering, consists of pre-cambering a part or parts during the weld process. This is a strategy used by Caterpillar for distortion control of their fabrications. This requires a change in boundary conditions at the end of the analysis. This has been implemented and validated.

5.3.4 Future Enhancement Material Law 'Annealing' Feature (Dynamic Strain Recovery)

One of the weaknesses of all computational weld modeling programs to date is that prediction of the final plastic strains is not as accurate as desired in regions of the weld where material annealing has occurred. When a weld pass is laid near another weld pass, the prior pass may partially re-melt. This is handled within computational weld codes using an 'annealing' approach where the history is removed in this element. VFT® currently uses a progressive annealing feature where a start temperature to an upper temperature usually chosen to be melting is removed [6]. This works well from a practical engineering standpoint and solution stability standpoint but could be improved if accurate plastic strains in these regions are desired. Some new work at Oak Ridge National Laboratory [7, 8, 9] involved working on a 'dynamic recovery' model that is more appropriate for modeling this. This is one of the tasks that will be considered in continuing work.

5.3.5 Future Stress Mapping Procedure

Mapping of stresses (and other internal variables such as strains) from the finite element mesh that is used for the weld analysis to a mesh that is used for crack analysis is often necessary in order to perform the subcritical crack growth analysis. This is conveniently performed in ABAQUS and this feature will be added to WARP3D using an existing Emc² mapping FORTRAN code. This is also one of the tasks that will be considered in continuing work.

5.3.6 Subtask 3.6 – Natural Crack Growth

The modeling of 'natural crack growth', whereby the crack is grown uniquely at every point along the crack front, is currently being performed by using an Emc² internal mesh generator called PipeFracCAE© (Emc² owned). This subtask involves tying the mapping procedure (Section 5.3.5) to the meshes produced by the FEAM code and PipeFracCAE©. This is essentially a 'place holder' for future work on the VFT® system.

5.4 System Port to AweSim OSC HPC Portal

Three important aspects of professional software development are project management, code collaboration, and a formal testing procedure. The procedures used for the VFT development program are summarized below.

Project management: Project management continues to be coordinated through the Basecamp website allowing for different teams to hold discussions, collaborate on documents, assign tasks, and check due dates. The Basecamp website (www.basecamp.com) is the preferred medium for project discussion, collaboration, and general discussion. This allows effective communication between the respective development teams in understanding and reaching project goals.

Code collaboration: The popular code repository hosting service GitHub (git.com) was used to collaborate on code development for the individual modules. It offers a variety of features such as code collaboration, reviewing, bug tracking, and version control that makes team development more dynamic and productive. Testing needs to be implemented before any changes to the code for a given module is pushed up to the production environment. As Emc^2 staff applied patches or pushed new features to an existing module the resulting software underwent a set of rigorous automated tests before being made available to the AweSim app store.

Formal testing procedure: A set of well-documented and well-vetted automated tests were necessary in the software development lifecycle for VFT to be a successful code. Testing needed to be implemented before any changes to the code for a given module is pushed up to the production environment. The latter half of the project focused on rigorous automated tests before making VFT® available to the OSC AweSim app store.

5.4.1 Software Components

Figure 65 shows the software components of the overall VFT® scheme. The user generates a weld-specific finite element mesh by their preferred mesher. However, a library of some simpler type meshes will be available to the user later including pipe and plate type weld meshes. These basic meshes are also available for download (see Section 3.2) to the user to aid in the development of more complicated meshes. Ordinarily a compatibility layer utility is undesirable because it imposes a time penalty on execution, but it is acceptable here because preprocessing is an interactive process without complicated computational needs.

Furthermore, it expedited migration of VFT to OSC. The Weld GUI (WGUI) project was originally engineered as a 32-bit Windows application using the defunct C++ compiler Borland CodeGear that hindered the migration to the OSC HPC environment. Many worthwhile steps were taken to successfully transition the Windows based Weld GUI to a Linux environment that users could connect to remotely and easily assimilate into their cloud based VFT workflow.

The first step relates to a common code compiler. The WGUI source code is now ported and is compiled under the latest adaptation of the previous defunct compiler, now called Embarcadero C++Builder XE7. With the compiler being accessible by both teams along with the GitHub version management tool, this now allows both teams to develop the GUI tool concurrently and in conjunction in their respective environments as improvements are made. On top of that, using a more recent compiler allows for the GUI to be compiled under a 64-bit environment, making it more compatible with OSC HPC systems.

The second step involves WINE. The open source WINE project is used to demonstrate the ability to run the Windows-based WGUI on the OSC HPC Linux-based environment. This was initially the biggest roadblock in the VFT integration project to the AweSim store. Not having to rewrite the Weld GUI for a Linux-based environment dramatically pushed forward the system port to the HPC cloud.

The third step concerns post processing. Currently OSC offers a variety of visualization software as well as desktop environments through a remote VNC solution to researchers, students, and other organizations. Accessing the Weld GUI remotely using OSC HPC resources through a VNC session was effortlessly demonstrated using the already available VNC server software. The preferred post-processing and visualization uses ParaView as discussed earlier. Several of the existing prototype AweSim apps utilize ParaView to present results either via scripted extractions of still images and animations or via a complete user interface to ParaView that is provided via a Java-based VNC client connecting to OSC's systems.

Usage accounting is the fourth step. An innovative batch system is currently being launched on the OSC HPC systems specifically geared to recording the resource usage of visualization software used through a VNC session (e.g., the Weld GUI or ParaView) for accounting purposes. Integrating this new batch scheduler into the system interface layer of the App Kit has recently been accomplished. This will in turn allow for a full usage accounting report of a given user whether it is through a remote VNC session or through an interactive web app.

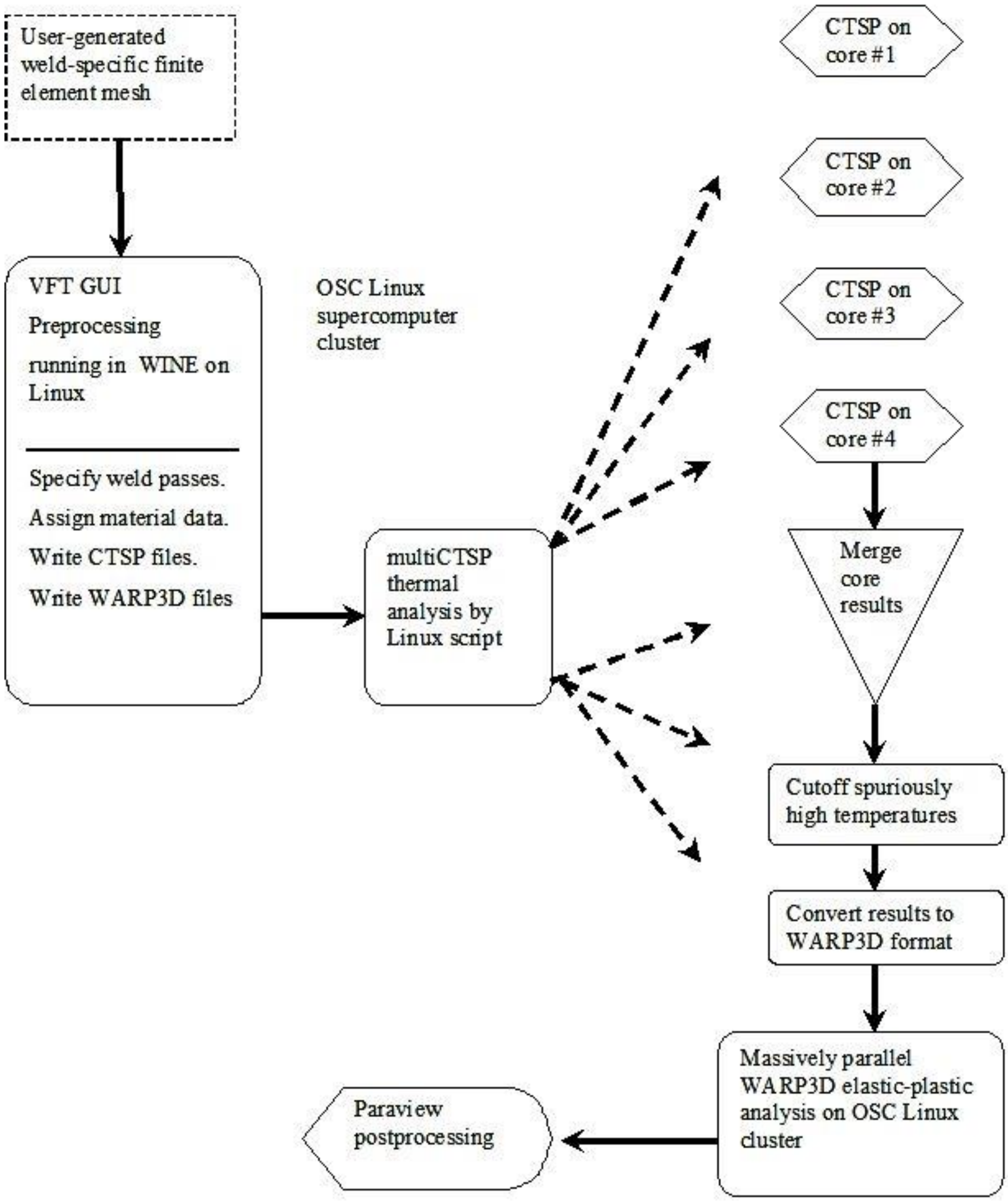


Figure 65 Software components of VFT on HPC cluster

5.4.2 CTSP Thermal & WARP3D structural solutions

The core thermal and structural solvers are Linux-based workflows that can be easily incorporated into OSC's HPC systems. WARP3D in particular takes advantage of the MPI library to fully utilize the capabilities of an HPC system. Both core solvers are successfully compiled using the OSC provided Intel Fortran compilers (Intel MPI Fortran compiler for WARP3D parallel) on the HPC cluster. In all cases the HPC builds of the respective solver successfully demonstrate reproducibility of all tests that were supplied and vetted by the Emc^2 developers.

Batch scripts are essential for simplifying the multi-program execution of VFT from the user's perspective. For CTSP, the multiCTSP script launches CTSP on each of the various cores, merges the results, deletes intermediate files, applies a cutoff for spuriously large temperatures, and converts results to WARP3D format (Figure 15). There are two such batch scripts for WARP3D that implement the serial build for a single node and the parallel build that utilizes the full capabilities that OSC has to offer. These scripts are documented in the corresponding GitHub wikis for their respective solver that allow for the given solver's workflow to be completely automated on an OSC HPC system from start to finish without user intervention.

5.4.3 Developer documentation

Thorough documentation is provided for the build process as well as the job submission process for both core solvers running on OSC HPC systems and is currently accessible through the shared GitHub project wiki. Current and future developers can follow as well as contribute to the step-by-step procedures of building the respective code on OSC systems to submitting it to the OSC cluster batch systems. Special care was taken with the WARP3D documentation outlining both the building and execution procedures for the OpenMP serial as well as the OpenMP+MPI parallel builds. Other documentation and tutorials are in progress. The user can download pertinent material as discussed in Section 3.2.

6 EDUCATIONAL TRAINING AND OUTREACH

An important effort with the VFT development on the AweSim OSC portal included outreach and education to small- and medium-size enterprises (SMEs) focused on presenting the advantages of VFT® and training on use of the system, including tutorials.

6.1 Education, Training, and Outreach of VFT®

During Phase II, we conducted outreach and education to SMEs on VFT® advantages and training/tutorials on use of the system. Tacit in the effort was to enlist SMEs who demonstrated interest in use of the code to enhance processes used in manufacture of their products. We worked with OSC staff on initial efforts to contact potential code users. OSC has recently created an accessible, open source "manufacturing app" format via the AweSim engagement program. AweSim is a series of web-based "app stores" designed to address manufacturing issues in a range of products through advanced modeling, analysis and simulation tools. VFT® has been implemented on the OSC "app store".

6.1.1 Outreach Strategy

In Phase II we expanded the survey conducted prior to Phase I to selected regional SMEs to determine interest in use of VFT® to achieve improved processes in fabrication of their products. OSC staff conducted an expanded survey during the spring/early summer of 2014 as part of their AweSim program.

6.1.2 Expanded Survey to Identify Potential Users

The National Center for Manufacturing Sciences (NCMS) with assistance from the Michigan Manufacturing Technology Center (MMTC) performed this expanded survey during 2014. OSC staff engaged NCMS/MMTC to use their survey experience as a starting point for an expanded survey. The expanded survey included assistance from Manufacturing Extension Partnership (MEP) Centers in Ohio, viz. Magnet (Cleveland) and TechSolve (Cincinnati). Results of the survey identified over 25 regional SMEs with interest in analysis and simulation tools in product manufacture that also employed welding in fabrication. Ohio regions where the SMEs reside include Cleveland (Northeast Ohio), Cincinnati (Southwest Ohio), Columbus (Central Ohio), and Dayton (Western Ohio). Initial contacts via email were made with 20 members of this SME group in December 2014 and follow up discussions were conducted in early 2015.

6.1.3 DOE Outreach Assistance Program

We also worked with DOE assigned commercialization assistance company, DAWNBREAKER, and assigned Business Acceleration Manager to assist in initial outreach and information activities with potential users of VFT®. DAWNBREAKER provided support in 1) Development of Network Contacts and 2) Primary Market Research:

Development of Network Contacts -This service involved identifying at least 20 contacts as potential users of VFT®. This was accomplished and supplemented by a list of general industry organizations. From here, 5 to 10 individuals were interviewed and a report was provided. This established members of a "core/seed" group; a collection of representatives of the regional manufacturing community and potential leaders of a transition to Digital Manufacturing. The seed group served as a test group for use of VFT®.

Primary Market Research - This service created a market research report based on information from direct customer contacts. This report listed 5 organizations with significant interest in use of VFT® who also showed interest in serving on the seed/core group.

6.1.4 Integration of User Training and Code Accessibility

The selected seed group was formed in summer 2015. This timing allowed the seed group to be established and introduced to the code. We delayed introduction/training until this time frame because the adapted version of VFT®, implemented as an "app", provides significantly more user friendly environment for training. This is consistent with the SBIR goal to provide HPC based technical tools that are accessible, affordable and do not require users to be an experts in technical details to effectively use the tool.

6.1.5 Preliminary Introduction and Training in Use of Code

Through discussions with SMEs in Phase I, extensive education and training in virtual design and analysis methods resident in VFT® is necessary because these firms lack knowledge/experience in such methods. These same SMEs had real interest in this methodology because of problems they face in fabrication of current products/structures. To provide access to a wide range of users and prior to establishing the seed group, we initiated the following preliminary activities:

- Discussions with 3 local to Columbus, Ohio SMEs to enlist their interest in use of VFT® while VFT® was being adapted for residence on OSC as an AweSim app.
- We identified the time frame to begin training in use of the code with these SMEs and we solicited and received "example problems" from their respective work places.
- This strategy accomplished the following goals: (i) Increased confidence in VFT® use and its effectiveness (ii) Provides early Beta testing to evaluate user friendliness/code performance on

OSC web-site, (iii) Identifies code improvements (e.g. GUI effectiveness) and utility of OSC residence and (iv) Enlist members to form the “core/seed” group.

These activities were provided to local SMEs at no cost for training, use of code as a VFT® app, and other related efforts. Our plans for achieving widespread use of VFT® beyond Ohio are based on having access to other MEP centers (over 60 in the U.S.) to aid in establishing seed groups in other states. As noted above, our team is equipped with a technical tool validated through users trained in its use on a system readily available for use by a wide range of SMEs at the end of Phase II.

6.1.6 Additional Outreach Activities Conducted in Phase II

Conference Presentations:

Brust, F. W., “Use of HPC Technology for Manufacture of Welded Structures”, ICCES (International Conference on Computational & Experimental Engineering and Sciences), Reno, NV, July 2015.

Brust, F. W., “Computational Weld Modeling Trends for Residual Stress with Applications in Industry”, AWS-Industry Conference, Lehigh University, Bethlehem, PA., August 2015.

Brust, F.W., “Federal Funding Opportunity: Adapted Version of VFT as App on OSC AweSim Platform”, International Industry Supercomputer Workshop (IISW)”, Cleveland, Ohio, October 2015.

Twombly, E. K., “Virtual Weld Simulation in a HPC Environment”, State Users Group (SUG) Conference, Ohio Supercomputer Center, Columbus, Ohio, December 2015.

Computational Weld class lecture at Ohio State University. Dr. Brust provided a guest lecture and demo of the VFT® system. Plan is to continue on a yearly basis. This will help market the code when these students get jobs in industry who will suggest using VFT® as needed.

6.1.7 Preliminary Informational and Educational webinar

As part of our outreach activities, we conducted a preliminary webinar at OSC in August 2015. Technical staff from Emc^2 and OSC conducted this activity. An initial group of SMEs was identified through emails, phone calls, and interviews. Staff members from each of 3 local organizations attended the webinar presentation on-site at OSC. (See picture below). Staff members from the non-local organizations attended remotely. Goals of this webinar were to review and evaluate methods employed in conducting the presentation regarding ability of attendees to understand technical content and determine level of interest in pursuing further training in use of the technology at their workplaces

A notable take away from the webinar was that little experience existed for use of digital tools in product manufacture for the participating SMEs. However, this same lack of experience was revealed in earlier conversations with SME’s in general and also was pointed out in the Primary Market Research Report conducted by DawnBreaker. Further, it was clear that the process involved in use of VFT® for design and analysis of welded parts/structures was understood by the participants. The steps prior to and after model creation were well understood. Nonetheless, accessibility has been achieved in Phase II by porting VFT® as an App to the AweSim Platform at OSC. The user does not have to invest in high end computational assets because the tool is available via the AweSim App to his/her work place. Also, inexpensive access has been achieved by allowing a flexible plan for a part time user (pays for hourly, weekly, monthly use on graduated basis) or as a more dedicated user that pays a nominal (yearly) fee.

The final goal, easy-to-use, has been partially satisfied because the ability to access the tool and menu driven nature of the GUI and subsequent automated and seamless solution process (push a button for next step style) allows for rapid and easily achieved results.

We also conducted initial educational and training sessions (3-full days) at OSC during March 2016 with the same 3 local SME organizations as noted above; they attended the sessions on-site at OSC. Likewise, the 2 non-local organizations attended the sessions remotely via a webinar. The training sessions were very successful for those participating in the sessions (for SMEs, Emc^2 and OSC staff members alike). This initial core group participated in solving example problems on VFT® and became efficient in use of the digital tool on AweSim by the end of the 3-day event. The training sessions did reveal that these first time users of VFT® on AweSim had little experience in finite element (FE) based methods and, correspondingly, almost no experience in creating the FE weld model required to correctly analyze and accurately solve a weld problem. This situation (little experience in FE based methods) was identified early on in our outreach/contact with potential SME users. The ability to generate an effective FE model is critically dependent on ability to create the appropriate FE mesh for the weld model. This deficiency (creating a FE mesh) was constantly pointed out during the training sessions by the participants. So, the need to address this issue was a much discussed subject during training.

The inability to create a weld model (generate FE mesh) is a pervasive matter and is not peculiar to this DOE SBIR program. This has been an ongoing issue with owners of other AweSim Apps. In order to partially accommodate this issue, Emc^2 has been using a "man-in-the-loop" approach. That is, in cases where the SME user has difficulty in creating an effective FE weld model mesh, Emc^2 and OSC staff have assisted in generating an appropriate weld mesh model and this has worked adequately so far. However, this assistance has been free of charge to date for our SME clients because we have been funded through Phase II when these situations have occurred. So beyond end of Phase II, we will provide a Fee-For-Service charge for this effort (assist in creating FE weld mesh) which is inconsistent with the goal of having an accessible, **low cost**, and easy to use digital tool to solve their problems. We currently have a weld mesh model assistance module available for VFT® users on AweSim but this added capability only includes simple weld models (e.g. fillet, lap, butt, etc.). More difficult welds (multi- pass, complex geometries, etc.) require assistance for the SME client set.

6.1.8 Additional Educational Training/Outreach for VFT® @ OSC

We continued to work with VFT® SME users through training and problem solving sessions on the AweSim Platform through the remainder of Phase II. Also, we enlisted experienced weld modelers from non-small organizations during the latter part of Phase II to use VFT® in order to solicit expert feedback on the process. We invited experienced weld modelers to use the VFT® AweSim App for two basic reasons; 1) to determine the degree of weld modeling efficacy resident in the adapted version of VFT®, and 2) to establish a user group consisting of core SME members and experienced weld modelers to create a projected ongoing revenue stream at the time of actual launch of VFT® as an AweSim App.

As it turns out, the VFT® digital tool is the first App on the AweSim Platform to be available to users from the manufacturing/fabrication sectors; the other current 4 to 5 AweSim App s will be launched at later dates. As such, this first App launch will be a learning experience for OSC staff, App users, Emc^2 staff, and other interested organizations to gage utility, efficiency, and focus of virtual analysis and design methods to improve processes in the manufacture of products.

But to continue the success of the VFT® App, we must expand our outreach efforts. As has been discussed in Phase I and Phase II reports and proposals, enlisting users of VFT® from the SMEs base is not a simple task. Outreach efforts in Phase II (through emails, phone calls, and, to a limited extent, visits) demonstrated clearly that face-to-face and webinar meetings are superior interaction modes to determine interest level and willingness to participate in training sessions, either on-site or remotely, through OSC. We plan to arrange face-to-face interactive discussions and webinars with potential SMEs as this work continues past Phase II completion. This face-to-face activity was definitely confirmed as highly desirable through conduct of Phase II. Also, we need to work deeper with the Ohio Manufacturing Extension Partnership (MEP) Centers and the Ohio Manufacturers Association (OMA) during the time after Phase II.

We used the Ohio MEP Centers early in Phase II to aid in identifying potential users and will again use the Centers and OMA to identify gatherings (conferences, meetings, etc.) of manufacturing organizations in the region (Ohio and close by neighboring states) so that we can attend and arrange face-to-face discussions with selected SMEs. Because initial direct contact efforts will be regional, we expect to accomplish the desired interactions within a 2-day period, some a one day event, to minimize travel costs. Additionally, our Phase II experience has shown that for SMEs that express interest in the technology, it is preferable to have technical personnel visit their work place and demonstrate utility of VFT® on a specific problem. This on-site visit and subsequent problem solution turned out to be the convincing item for enlistment in use of the tool. It is highly likely that face-to-face discussions at selected gatherings will be followed by on-site visits to SMEs. We intend on working with the OMA and MEP centers to generate lists of organizations to make travel and attendance time-wise efficient. We may also find it worthwhile to have a "trade booth" at the gatherings to display VFT® information.

At a minimum, we will provide brochures, other hand outs, etc. at these meetings to assist in discussions and create the atmosphere for questions pertaining to VFT® while emphasizing goals of improved fabrication processes for products using VFT®, viz. accessible from work place, low cost, and easy to use. The main purpose of this outreach is to inform, educate, and create users of the technology so that use through the AweSim Platform generates an income stream to perpetuate/spread throughout the U.S.

We worked with DAWNBREAKER to create a brochure to aid in the discussion purposes. Some of the organizations we worked with are listed in Table 1.

Table 1 SMEs Contacted by Emc^2

Regional SMEs				
Company Name	Contact	Contact Email	Location	Phone Number
Peerless Foods	Jason Switzer	jswitzer@peerlessfood.com	Toledo, OH	937-494-2803
Enginetics	Gary Thompson	gthompson@enginetics.com	Dayton, OH	937-754-3223
AFTCO	Chris Van Raalten	vanraaltenc@aftco.com	Charleston, SC	216-246-5933
Beckett Corp	Greg Bloomfield	gbloomfield@beckettcorp.com	Cleveland, OH	440-353-1332
Midway Products	Earl Bledsoe	Earl.bledsoe@midwayproducts.com	Monroe, MI	419-303-1233
Dayton-Phoenix	Mike Ayette	mayette@dayton-phoenix.com	Dayton, OH	937-496-3962
Ethicon Endo, Div of J&J	Jerry Morgan	jmorgan@eesus.jnh.com	Cincinnati, OH	513-337-7324
Stock Equipment	Jeff Mattern	Jeffery.mattern@stockequipment.com	Cleveland, OH	440-543-6000
Fives Group	Dennis Quinn	Dennis.quinn@fivesgroup.com	Cleveland, OH	216-271-6000
SIFCO	Gary Wilson	gwilson@sifco.com	Cleveland, OH	216-219-2374
Tyco Electronics	David Falquette	David.falquette@tycoelectronics.com	Cleveland, OH	419-521-9566
Swagelok	Joel Feldman	jfeldman@swagelok.com	Cleveland, OH	440-649-3531
Thogus	Greg Werner	gwerner@thogus.com	Cleveland, OH	440-993-8850
PDSI	Kevin Sizemore	ksizemore@P-D-S-I.com	Dayton, OH	937-866-3377
Worthington Industries	Alex Spires	Alex.spires@worthingtonindustries.com	Columbus, OH	614-438-3145
Ferry Industries	Bruce Karem	bkarem@ferryindustries.com	Stow, OH	330-923-7237
E-CI	Rick Neff	Rick.neff@e-ci.com	Cincinnati, OH	513-367-7663

HDT Global	Ben Bullen	Ben.bullen@hdtglobal.com	Stow, OH	216-433-6202
Regional SMEs, cont'd				
KTH	Aaron Doak	Aaron.doak@kth.com	St. Paris, OH	937-663-9321
Fecon	Dennis Goldbach	dgoldbach@fecon.com	Cincinnati, OH	513-254-1447
Local SMEs Enlisted by Emc^2				
Worthington Industries	Elvin Beach	Elvin.beach@worthingtonindustries.com	Columbus, OH	614-438-3212
Uni-Facs	Chris Grimm	cgrimm@unifacs.com	Columbus, OH	614-274-1128
Regional SMEs Contacted by OSC				
Bird Technologies	John Winter	jwinter@birdtechnologies.com	Solon, OH	440-519-2358
Henny Penny	Ed Forkey	eforkey@hennypenny.com	Eaton, OH	937-456-8669
Henny Penny	David Norris	dnorris@hennypenny.com	Eaton, OH	937-456-8790
Henny Penny	Ed Phillips	ephillips@hennypenny.com	Eaton, OH	
Norlake Mfg	James Nunamaker	Jim.nunamaker@norlakemfg.com	Elyria, OH	440-353-3200

7 SUMMARY

This report summarized the progress made on the US DOE Small Business Innovative Research Funding Opportunity Number DE-FOA-0000760 grant on 'Adoption of High Performance Computational (HPC) Modeling Software for Widespread Use in the Manufacture of Welded Structures' made to Engineering Mechanics Corporation of Columbus between April 16, 2014 and August 30, 2016.

Emc^2's DOE SBIR Phase II effort has successfully adapted Emc^2's Virtual Fabrication Technology (VFT®) weld simulation program to perform efficiently in a high performance computing (HPC) environment independent of commercial software on a platform to permit easy and cost effective access to the code. These efforts provide the key for small and medium (SME) sized companies to have access to a sophisticated and proven methodology that is quick, accurate and cost effective and available "on-demand" to address weld-simulation and fabrication problems prior to manufacture. This access route will permit SMEs to perform weld modeling to improve their competitiveness at a reasonable cost.

VFT® is a sophisticated, mathematical and physics-based computer code system that simulates the weld process. The weld process is a highly non-linear and difficult phenomenon to capture which involves melting, removal and re-depositing of material, continuous deposition of new weld material, and annealing in the heat affected zone. Prior to Emc^2's DOE SBIR Phase I award, VFT® exclusively employed a commercially available software code as the system solver. As such, the user was required to have a license for this commercial code (pay a fee) to solve the welding problem via VFT®.

In order for small- and mid-size manufacturing and engineering firms to have access to a version of VFT® that is cost effective and efficacious for their manufacturing problems where welding is a major part of their fabrication process, we are enhancing VFT® by permitting simple access on a cloud computing platform hosted at the Ohio Super Computer Center (OSC) on their AweSim App platform.

After extensive testing of the system to ensure the system was stable the system was made available for use on April 1 2017. Continued improvement will be made to enhance the system based on user needs in the coming years.

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