CHALLENGES IN VERIFICATION OF CWM SOFTWARE TO COMPUTE RESIDUAL STRESS AND DISTORTION IN WELDS

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ABSTRACT
Validation of a Computational Weld Mechanics (CWM) code for a particular welding application requires an estimate of the difference between experimentally measured parameters and parameters computed by a computational model. This requires estimates of the uncertainty in both the experimental data and the computational data and this requires careful design of both the experiment and the CWM model. The authors experience in performing validation tests for a Computational Weld Mechanics (CWM) code is summarized. An example of a validation test for a welding application that compares measured and computed transient temperatures, displacements and strains is described in detail that demonstrates that model can accurately predict this data. Challenges on both the experimental side and computational side are discussed but the greatest challenge is the limited availability of experimental data that has a measure of uncertainty.

INTRODUCTION
Arc welding is a complex manufacturing process in which an electric arc generates heat in an area approximately one cm² while travelling at speeds of approximately 1 to 5 mm/s to form a pool of liquid metal with volume usually slightly less than 1 cm³. As the liquid metal on the trailing edge of the weld pool solidifies, a weld joint or weld overlay is created. The transient temperature field drives metallurgical phase changes, thermal expansion-contraction and changes temperature dependent properties of the materials. The microstructure evolves as it is heated and cooled with phase changes, annealing, recrystallization and grain growth. The strain due to thermal expansion-contraction, phase changes and restraint of the structure and fixtures generates stress and plastic deformation. The plastic deformation leads to residual stress and deformation.

The physics and mechanics of welding can be separated into the physics of the arc and weld pool on the one hand and the physics of the solid on the other hand. The physics of the arc and weld pool primarily involve magneto-hydrodynamics and fluid flow with length scales less than 1 mm and time scales less than 0.1 second. The physics of the solid primarily involve solid mechanics with length scales greater than 1 mm and time scales greater than 1 second. The coupling between the physics and mechanics of the weld pool and the physics and mechanics of the solid is almost entirely though the thermal analysis in the solid. The heating effect of the arc and weld pool can be modelled by parameterizing a power density distribution function with net weld power and the weld pool shape, size and position as a known function of time [1]. These weld pool parameters shape and size parameters are usually estimated from macro-graphs of cross-sections of the weld joint.

A computer model to predict the behaviour of this complex process can save time, money and explore ‘what if’ scenario’s that are difficult to assess by experiment. The arguably best models of the welding process, solve the conservation of energy, mass and momentum, i.e., three coupled partial differential equations, with realistic 3D geometry of the structure and the welding process and the most realistic constitutive equations and weld process models available. Because the welding process is
transient, non-linear and usually involves complex geometry, the best model are based on 3D transient non-linear Finite Element Analysis (FEM). Because such models require complex numerical algorithms and sophisticated software, the first models did not emerge until the 1980s. Current models often have have 10K to 200K 8-node brick elements and are often solved for thousands of time steps. Reference [2] is good reference on the state of the art of CWM as it emerged in 1985. References [3] and [4] discuss progress in CWM in 1995 and 2008 respectively that has contributed to the development of CWM. VrWeld is largely based on research led by Professor John Goldak’s research in computational weld mechanics.

The essence of the validation process is the comparison of the output or prediction from a computational model with the output or measurements from a set of experiments. To make the discussion definite in this paper, we will compare in some detail the measured and predicted an experiment described by Masubuchi [5] and the predicted values by VrWeld [6]. In this case, variables to be compared are the transient temperatures measured by four thermocouples, the transient longitudinal strains measured by four strain gauges and the transient displacement measured by one displacement gauge.

1 Computational Weld Mechanics as a Control Problem

Computational Weld Mechanics (CWM) can be viewed as a control problem that has a state vector and a control vector. The state vector represents the, geometry of the structure, the transient temperature, displacement, strain and stress fields and the evolution of microstructure. Associated with the state vector are the constraint equations that conservation of mass, momentum and energy and the constitutive equations associated with material properties which are functions of temperature and microstructure. The control vector has parameters such as weld power, weld speed, the distribution of power density near the arc and the position of the arc. The control vector is a function of time.

In validating a CWM software program, it is useful to distinguish between errors in the state vector and errors in the control vector. If one changes the control the vector, one is modelling a different weld.

The input data to VrWeld are:

1. The 3D geometry of all parts and fixtures in the structure to be welded are usually imported as Stereolithographic (STL) files. If the 3D transient geometry of each filler metal pass is not provided as STL files, then it must be modelled and the data for the geometry of the filler metal models must be provided.
2. The composition, temperature dependent thermal and mechanical material properties for each alloy type for each part in the structure including filler metal of welds must be specified.
3. The weld process parameters including weld current, weld voltage, power density distribution in the weld pool are needed. For a MIG welding process the filler metal wire size and speed are needed. The start time and start position of each weld pass and the speed as the arc travels along the weld path is needed. The delay time between the end of one weld pass and the start of the next weld pass is important.
4. If fixtures are applied or released, the appropriate time dependent boundary conditions must be defined to model the action of each fixture.
5. A cool-down time after the welds have been completed is chosen to allow the structure to cool to room temperature.
6. The initial state of the temperature, microstructure and strain or stress is needed. Often the initial state of the temperature is the ambient temperature; the initial state of strain and stress are assumed to be zero tensor fields but any known initial state can be applied.
7. If sensors such as thermocouples, strain gauges, displacement transducers, residual stress sampling volumes are of interest, then the position and the times of interest of each transducer should be specified as a virtual sensor.

The output data from VrWeld include the following fields:

1. Transient temperature field.
2. Transient displacement field.
3. Transient elastic, thermal, plastic and total strain vector or strain tensor field.
4. Transient stress and deviatoric tensor field and principal stress fields as scalars or vectors.

1.1 What Equations Does VrWeld Solve?

1.1.1 Conservation of Energy or Heat Equation

With specific enthalpy \( h \), thermal flux \( q \) and a power density function \( Q \), temperature \( T \), temperature gradient \( \nabla T \), thermal conductivity tensor \( \kappa \), specific heat \( c_p \), the heat equation can be be written in the following form:

\[
\begin{align*}
\dot{h} + \nabla \cdot q + Q &= 0 \\
q &= \kappa \nabla T \\
\frac{dh}{dt} &= c_p dT.
\end{align*}
\]

VrWeld solves this time dependent system of partial differential equation on a domain defined by an FEM mesh. The domain is dynamic in that it changes with each time step as filler metal is added to the weld pass. The initial condition is often assumed to be a constant temperature of 300 K but the domain can be initialized to any initial temperature field. The material properties \( \kappa \) and \( c_p \) are usually temperature dependent. The heating affect
of the arc is often modelled by a double ellipsoid power density distribution that approximates the weld pool as measured from macro-graphs of the cross-section of several weld passes [1]. However, many other weld pool models can be used. A convection boundary condition \( q = h(T - T_{amb}) \) usually is applied to external surfaces. The FEM formulation of the heat equation leads to a set of ordinary differential equations that are integrated in time using a backward Euler integration scheme.

1.1.2 Conservation of Momentum Equation
Given the density, \( \rho \), the elasticity tensor as a \( 6 \times 6 \) matrix, the body force \( b \), the Green-Lagrange strain tensor \( \varepsilon \), VrWeld solves the conservation of momentum equation that can be written in the following form in which inertial forces \( \rho \ddot{x} \) are ignored.

\[
\nabla \cdot \sigma + b = 0 \\
\sigma = D\varepsilon \\
\varepsilon = (\nabla u + (\nabla u)^T + (\nabla u)^T \nabla u)/2
\n\]

VrWeld solves this partial differential equation for a viscothermo-elasto-plastic stress-strain relationship using theory and algorithms developed by J.C. Simo and his colleagues [11]. The initial state often is assumed to be stress free. However, if the initial stress state is known, it could be initialized in VrWeld. The Dirichlet boundary conditions constrain the rigid body modes. The system is solved using a time marching scheme with time step lengths of approximately 1 second during welding and usually an exponentially increasing time step length after welding has stopped. See [12] and [13] for more details on stress analysis of welds.

1.2 Guidelines for verification and validation for use in an Application

The Preface of the ASME standard [7] states: This document provides general guidelines for implementing V&V of computational models for complex systems in solid mechanics. The guidance is based on the following key principles:

1. Verification (addressing programming errors and estimating the numerical errors) must precede validation (assessing a model’s predictive capability by comparing calculations with experiment).
2. The need for validation and the associated accuracy requirements for computational model predictions are based on the intended use of the model and should be established as part of the V&V activities.
3. Validation of a complex system should be pursued in a hierarchical fashion from the component to the system level.
4. Validation is specific to a particular computational model for a particular intended use.
5. Simulation results and experimental data must have an assessment of uncertainty to be meaningful.

Although the state of the art of V&V does not yet lend itself to writing a step-by-step performance code/standard, this guide provides the computational solid mechanics (CSM) community with a common language and conceptual framework to enable managers and practitioners of V&V to better assess and enhance the credibility of CSM models. Implementation of a range of V&V activities is discussed, including model development for complex systems, verification of numerical solutions for governing equations, attributes of validation experiments, accuracy requirements, and quantification of uncertainties. Remaining issues for further development of a V&V protocol are identified.

An overview of the process of verification and validation is shown in Fig. 1.
1.3 Verification of VrWeld

Verification of VrWeld software is done by comparing results computed by VrWeld with relevant mathematical problems for which the exact solution is known. (Occasionally when mathematical problems with exact known solutions are not available, numerical solutions that are considered to be highly accurate are sometimes used.) This is done for all mathematical equations in the model. Goldak Technologies Inc. (GTI) does verification by creating ‘Test Suites’ that are collections of problems for which the exact solution is known for a particular solver such as the solver for the transient heat equation or the solver for transient visco-elastic-plastic stress analysis. When these test problems are run, the sum of squares error in the solution of each problem is reported. This report is generated automatically and sent by email to the appropriate software developers at GTI. These test suites of verification problems are run routinely.

1.4 Validation of VrWeld

Examples of validation are given in the references [9], [10], [4]. In [9] two examples are an overlay weld analysis with 27 weld passes in two layers covering a 100 × 100 mm block in a 400x400 mm square plate 30 mm thick and an overlay weld analysis with 51 weld passes in two layers covering a 200 × 200 mm block in a 400 × 400 mm square plate 30 mm thick. The experimental data was gathered from 6 thermocouples and 22 strain gauges. In addition, distortion was measured by a coordinate measuring machine and compared to computed distortion or displacement. The agreement between measured and computed data values was considered to be remarkably good. In [4], the transient displacement field was measured with a high precision stereo camera and compared with the transient displacement computed with VrWeld. Again the agreement was considered to be exceptionally good. In [10] the residual stress measured by neutron diffraction and x-ray synchrotron diffraction was compared with the residual stress computed with VrWeld. Again the agreement was considered good.

In all of these validation tests except [4], only one experiment has been done. As discussed in [10], [4] [7], it is desirable to conduct multiple experiments and use statistics to assess the accuracy statistics of the experiments. In the one case [3], where repeat experiments were available, the errors in the experiment were of the same order of magnitude as changes induced in the values computed by VrWeld by reasonable changes in the input parameters, e.g., 10% changes in weld power or weld speed.

The inputs to VrWeld are the geometry of the domain or structure, the temperature and microstructure dependent thermal and mechanical material properties, the initial conditions and boundary conditions. In Computational Weld Mechanics (CWM) the geometry of the filler metal added and the weld pool are important. The sensitivity of the computed solutions to errors in these inputs can be computed by solving the problem with variations in the inputs.

In all validation analyses performed by the authors to date, the initial state of the structure being welded has been assumed to zero initial stress and the geometry was the exact geometry of the original design. If estimates of the initial state or deviations from the original geometry were available, then ‘what if’ analyses could be run to estimate their effect.

In addition to errors in the inputs, truncation errors can arise because the mesh size or spatial discretization is finite and the time step size is finite. These truncation errors can be estimated by running analyses with a finer mesh or shorter time steps. The analyses have been done with linear FEM elements, i.e., 8-node bricks and 6-node prisms. The analyses could be run with either a finer mesh or with a mesh with higher order elements such as quadratic brick elements to obtain an estimate of the truncation error due to finite size of elements. Errors can also be bounded by using duality, e.g., the Prager-Synge Hyper-Circle theorem.

After running a first analyses, it can also be useful to identify and form a sub-project on a small sub-domain that has an above average error norm. Then mesh the sub-domain with a finer mesh and solve this small sub-domain with time dependent boundary conditions obtained from a previous analysis with a coarser mesh and possibly coarser time steps. If the sub-domain is smaller than the global domain, it is usually feasible to solve it with a much finer mesh and possibly much shorter time steps than the larger global domain.

2 Validation Process

The validation strategy that the authors usually use is summarized below. This assumes that welds have been made with several thermocouples, strain gauges and possible displacement transducers.

The authors acknowledge that it could be argued that the Validation Process as described below should be called a Calibration Process because the computational analysis has access to the experimental data. However, we are trying to develop a validation process that is accepted by people doing the welding, i.e., the welding community. When the requirements for designing experiments for weld validation tests are well understood by the welding community, then indeed, the computational model should be run without access to the experimental data.

2.1 Validation of Transient Thermal Analysis

Because the transient temperature field drives microstructure evolution and thermal expansion, it is critical that the transient temperature field be computed accurately. This is the first stage of the computational validation process. To do this, the authors usually follow the steps below.

1. Adjust the welding start time by matching the time of the first pass peak temperature at the first thermocouple;
2. Adjust the power by matching the peak temperature of the first pass at the first thermocouple;
3. adjust the welding speed by matching the time of the first pass at the peak temperature at the next thermocouple;
4. Re-adjust the power by matching the peak temperatures of the first pass in the first two thermocouples;
5. Adjust the start dwell time by matching the thermocouple peak temperatures of the first pass;
6. Adjust the convection coefficient function by matching cooling curves after the first pass in all TCs;
7. Adjust delay times after each pass by matching the times of all peak temperatures at all thermocouples;
8. In some cases, adjust the thermal conductivity.
9. Re-adjust the convection coefficient function by matching cooling curves after all passes finished in all thermocouples.

Possible improvements that might be required if the difference between measured and computed temperatures is not acceptable are given below.

1. Use different weld procedures for each pass (power, weld speed) and repeat steps 2 to 4.
2. Use different start dwell time for each pass;
3. Use decreased power at the end of each pass;
4. Change coefficients for each term in the convection coefficient function (we only played with the global scale);
5. Different convection coefficient functions after each pass.

2.2 Validation of Microstructure Evolution

The final microstructure can be measured on sections of a weld using metallographic techniques and compared with the computed microstructure. It can be useful to compare measured and computed hardness maps.

2.3 Validation of Transient Strain and Displacement Analyses

When the authors are satisfied that the transient temperatures and microstructure analyses are acceptable, then the focus turns to the transient displacements and strains.

One of the most important material properties for this stage is the temperature dependent specific volume or density for each phase in the microstructure. In low-alloy steels, ferrite, pearlite, austenite or gamma, bainite and martensite phases often play important roles. Since the microstructure in low alloy steels can be quite different on heating and cooling, the specific volume at each Gauss point is a function of both temperature and microstructure. This function is history dependent.

The temperature dependent yield stress and hardening modulus are important. Here again, the evolving microstructure makes this non-trivial. The authors prefer to specify the temperature dependent yield stress and hardening modulus of each phase separately. Then compute the temperature dependent yield stress and hardening modulus at a Gauss point by a rule of mixtures as a function of the fraction of each phase present and the temperature.

2.4 Sensitivity of Computed Results to Model Parameters.

The finite element mesh and time step size must be fine enough to be able to resolve transient temperature, microstructure and displacement fields with sufficient accuracy. Near the weld pool, the authors often use mesh sizes in the range of 1 to 10 mm. and time step size near 1 second.

3 A Validation Example

Masubuchi describes a careful experiment in [5] to measure the transient temperatures, deflection and strains in an edge weld on a 152 × 1220 × 12.5 mm bar of Aluminium 5052-H32. The transient temperature was measured by four thermocouples, the transient longitudinal strain was measured by four strain gauges and transient displacement was measured by one dial gauge and two extensometers. The position of each sensor is shown in Fig. 2. The sensor output data is given in the form of graphs. See Fig. 3, 4 and 5. The data from plots in [5]'s have been converted to tables by picking points from scanned images of the plots and importing the point coordinates into the the CWM analysis for comparison.

The temperature dependent material properties of Al 5052-H32 given in a plot in [5] were also converted to tables by picking points from scanned images of the plots. This data was used in the CWM analysis of this test.

The displacement boundary conditions for the test removed the rigid body modes by constraining the bottom left edge to zero displacement and by constraining the bottom right edge to zero transverse motion and zero vertical motion but to allow horizontal translation.

Figure 2. Specimen and locations of sensors and gauges [5].
The analysis was run with the welding parameters described in [5] for the experimental test. After running the first thermal and stress analysis, some steps were taken to adjust the input data to improve the agreement between measured and computed thermocouple results. These steps are explained in the following sections for thermocouples, strain gauges and dial gauge separately.

3.1 Validation of Transient Temperature Computation

There was no indication of arc weld efficiency given in [5] and therefore different values of arc efficiency were applied to match the peak temperatures measured by each of thermocouples. Figure 3 shows the result using an arc efficiency value of 60%. Values less than 60% shift the thermal profile below the experimental profile and the values greater than 60% shift the thermal profile above the experimental profile. The convection coefficient function was changed by scale factors of 0.5, 0.8, 1.2 and 1.5 and the changes in the transient temperature were not significant.

3.2 Validation of Transient Strain Gauge Computation

Figure 4 compares the computed result for strain gauges positioned as described in [5] with the experimental data taken from [5]. Thermal strain is fully subtracted from the total strain. Red, dark blue, light blue and black are experimental data for strain gauge 4, 3, 2 and 1 respectively. Green, magenta, yellow and light brown are computed results for strain gauge 4, 3, 2 and 1 respectively. There is a good agreement for strain gauges 1, 2 and 3.

However, the strain measured with strain gauge 4 is sensitive to the position of the strain gauge wrt to the weld fusion zone. In [5] the position of the strain gauge is given as a point. In fact, the strain gauge has finite size, possibly it is 10 to 15 mm long. It would have been better if [5] had specified the position of the strain gauge by the position of its corners. This sensitivity of strain gauge 4 to its position wrt to the weld is shown in Fig. 5. The results for strain gauge 4 positioned with distances from top edge of 4.13, 3.81, 3.49, 3.17, 2.85 mm are shown in green, dark blue, magenta, light blue and yellow respectively. Experimental data is shown in red.

As temperatures near the weld pool approach the melting, the material behavior changes from rate independent thermal-elasto-plastic to rate dependent or visco-thermal-elasto-plastic. When the metal melts the viscosity drops by many orders of magnitude. Because material property property data is usually not available for temperatures near the melting point, a cut-off temperature is applied in the stress analysis. This is a low pass filter such that temperatures sent to the stress solver that exceed this temperature are set to this temperature. To assess the sensitivity of the computed results to the value of the cut-off temperature, values of the cut-off temperatures were varied to temperatures very close but not equal to the melting point.
Figure 5. Sensitivity of strain gauge 4 to its position distanced from top edge by 4.13, 3.81, 3.49, 3.17, 2.85 mm are shown in green, dark blue, magenta, light blue and yellow respectively. Experimental data is shown in red.

In addition, the specific volume was perturbed by perturbing the coefficient of thermal expansion. Our tests shows that increasing the coefficient of thermal expansion (CTE) shifts the end tail of the transient displacement and drops the minimum. Fig. 6 compares the settings with cut-off temperature 850 K, convergence criteria 0.000001, maximum number of Newton-Raphson iterations10 and increases in the coefficient of thermal expansion by adding 2e-6 from the original temperature dependent values taken from [5]. This is an increase in CTE of about 10 %. The material for filler and body are Al-5052-H32 using the properties are taken from [5]. The CPU time for this analysis remains about 2500 seconds for this setting.

3.2.1 Adjustment for best agreement The best agreement is achieved using a cut off temperature of 850 K, convergence criteria 0.000001, max NR 10 and the coefficient of thermal expansion increase by 2e-6 using Al-5052-H32 material for filler metal and body with the properties taken from [5]. The CPU time for this analysis is about 2500 seconds for this setting. Figure 7 illustrates this result and the experiment for comparison.

4 Conclusion For Masbuchi’s test problem, the difference between the measured and computed transient temperatures, displacements and strains was sensitive to the value of the control vector.

Our experience in performing validation tests for Masbuchi’s test problem and for other test problems, suggest that greatest source of error is in specifying the control vector, i.e., the parameters that characterize the weld being made such as weld power, weld speed, start times, etc. Errors in geometry, i.e., the difference between the geometry specified in CAD files and the geometry of the real structure being welded can be significant. Once errors in the control vector have been reduced sufficiently, then errors in material composition, temperature dependent material properties and evolution of microstructure become important. These tend to be more important in the fusion zone and HAZ of the welds.

REFERENCES
Figure 7. Comparison the measured mid-length deflection and computed mid-length deflection with setting of cut-off temperature to 850 K, convergence criteria to 1e-6, maximum number of Newton-Raphson iterations to 10 and an increase in CTE by adding 2e-6 to the original CTE values taken from [5], see Fig. 2.