WARP3D: OPEN SOURCE SOFTWARE FOR 3D NONLINEAR FRACTURE MECHANICS

Robert H. Dodds, Jr.*

University of Illinois, Urbana, IL, USA
** Presenting Author email: rhdodds@gmail.com*

Abstract

The WARP3D project (warp3d.net) provides all source code, extensive documentation and ready-to-run executables on Windows, Linux and macOS for researchers and practitioners worldwide. Developed by a group at the University of Illinois starting in the late 1990s to support academic research, WARP3D capabilities focus on modeling nonlinear fracture processes primarily in metals from the microscale to structural components. This presentation describes the origin and several key capabilities of the code.

1. Overview

WARP3D grew from DARPA sponsored, computer engineering research in the late 1980s-early 1990s at the University of Illinois for parallel computing in engineering applications. Early versions of a small 3D FE code with limited capabilities provided a testbed to explore software architectures that best mapped FE computations onto rapidly evolving hardware designs. Once hardware designs stabilized in the late 1990s, a small group began adding fracture mechanics capabilities to support ongoing research. The benefit that graduate students, Post-Docs and collaborators derived from unfettered access to the entire source code for their work confirmed a decision to make the project, by then named WARP3D, open source with essentially no restrictions.*

The core design of WARP3D supports 3 levels of parallel execution: (1) Message Passing Interface (MPI) to process model sub-domains via partitioning distributed over nodes of supercomputer clusters, (2) domains assigned to each node partitioned into blocks of elements that are processed in parallel using threads via OpenMP, and (3) a structure of arrays (SoA) design (tinyurl.com/4tebkawe) at the element block level with long, stride-1 loops to enable efficient, automatic vectorization by compilers. Most all users now report running the code on laptop and deskside computers which today (2022) often have 10s of cores and 100s GB of memory – there by using levels (2) and (3) parallelism for their analyses. Nonlinear models with > 1M nodes-elements readily run in practical wall-times on these computers.

By: (1) limiting the focus to static/dynamic, (implicit) nonlinear stress analysis (no thermal, acoustic, electro-mechanical or coupled solutions), (2) providing only 3D solid elements (hex,tet), interface-cohesive elements, and link-bars, (3) adopting the Intel MKL (Pardiso) family of equation solvers, and (4) depending on other software for pre-post processing, *e.g.* Patran, FEMAP, FEACrack, ParaView, …, the code size of 1400+ routines remains comparatively small.

WARP3D enjoys widespread use in university and industrial settings. A key driver for success lies in the ready-to-use executables to perform analyses — no code building required. The web site received 6.5K page views January-August this year (2022) and averages ~300 unique visitors each month. Approximately 20% of visits originated from the USA, 14% from China, 14% from Germany; the remaining 52% of visitors originated from 76 other countries. Journal and conference citations (other than developer papers) number in the 100s, with most of those authors unknown to the developers. RHD routinely responds to email inquiries from graduate students and Post-Docs, nearly always about theoretical and modeling concepts in fracture rather than issues in using the code.

2. Some Key Capabilities for Nonlinear Fracture Modeling

The following capabilities implemented in the code support a wide spectrum of nonlinear fracture analyses. Some items have URLs for sections of the documentation.

a. A robust finite-strain formulation for solid elements and interface-cohesive elements using rotation neutralized rates based on polar decompositions of **F**.

b. Domain integral computation of J and interaction integrals (K_I - K_{II} - K_{III}, T-stress). The J-integral computation includes inertia, crack-face loading, temperature effects, functionally graded and anisotropic materials, initial-state framework for user-defined residual stresses and for thermo-mechanical processing before crack introduction. tinyurl.com/4ua7sj5v

c. 3D crack extension via: (1) element deletion governed by GTN model or SMCS models including multiple forms of Lode angle effects and mesh regularization features, (2) automatic node release at critical CTOAs or user-requested releases, (3) interface-cohesive elements. Adaptive tracking/control of crack growth quantities (porosity, plastic strain, CTOA, …) to minimize history discretization effects.

d. Integrate existing Abaqus UMAT, UEXTERNALDB, SIGINI routines with cosmetic changes.

e. Full Newton, incremental-iterative solutions with time-history integration, global displacement extrapolation, line search and automatic, adaptive solution strategies to enhance convergence, adaptive local constitutive updates to control truncation errors.

f. Nonlinear material models including viscoplastic and temperature effects; the GTN plasticity model for void growth (with rate and temperature effects), finite-strain plasticity including the effects of solute hydrogen on the micro-scale flow properties, an advanced model for cyclic plasticity of metals including nonlinear kinematic-isotropic hardening, more generalized complex cyclic behavior (Cottrell-Stokes) and temperature dependent cyclic properties; Norton-Bailey power creep.

g. A crystal plasticity material model for rate and temperature dependent simulation of microscale plastic flow in metals: fcc, bcc, bcc48, hcp6, hcp18, and a single slip system for teaching. A variety of rate and temperature dependent hardening constitutive models to couple shear-strain rates with shear stresses. Options for simple gradient-based geometric hardening incorporate the effect of necessary dislocations on hardening properties.

h. User defined multi-point constraints; absolute constraints in global and non-global coordinates; combine with link elements to impose general periodic boundary conditions. Tied-contact to connect topologically dissimilar but geometrically congruent meshes using automatically constructed multi-point constraints.

i. A forward translator program that generates WARP3D input files from Patran-style neutral files. WARP3D outputs simple flat files of node, element and material state results in text or stream formats. Builds an EXODUS II database (.exo) file for ParaView and other post-processors. tinyurl.com/522k39p4 and tinyurl.com/522k39p4

j. Extensive, self-checking suite of 160 verification problems. tinyurl.com/dauwcrtv

Acknowledgements
The contributions of many graduate students, Post-Docs and collaborators have made WARP3D a useful resource for researchers and practitioners (see User Manual for complete contributor list). Significant financial resources for fracture mechanics research and/or code support have been provided by: NASA (ARC, MSFC), USNRC, ORNL, Intel (via Ohio Supercomputer Center), Quest Integrity, Inc., Kinectrics, Inc., EMC2, DoD SBIRs, and graduate fellowships from NSF, DoE, NDSEG, ONR and the Newmark and Yeh endowments at the University of Illinois.