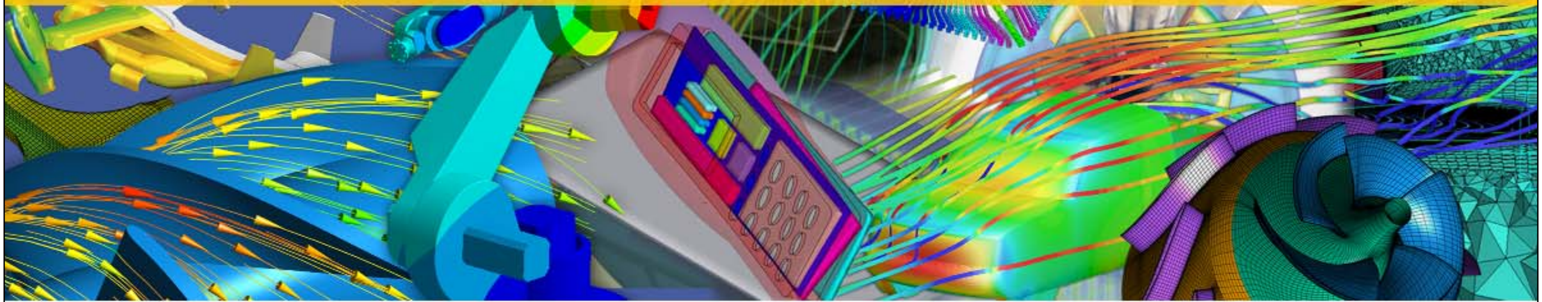
ANSYS®

POLYFLOW

Technical Specifications

3.11 RELEASE



POLYFLOW 3.11

POLYFLOW® is the unchallenged CFD solver for complex non-Newtonian rheologies including viscoelastic flow. The direct coupled solver using the finite element technique ensures a convergence to address the complexities of flows related to polymer processing and glass forming. Advanced techniques to deal with deforming mesh, complex motion of solid parts (screws) and detection of contact between free surface and molds are available to accurately simulate the many different processes involved in these industries.

This document summarizes the technical specifications and capabilities for POLYFLOW 3.11.

www.ansys.com

General Modeling Capabilities

- 2-D planar, 2.5-D planar (includes 3rd velocity component), 2-D axisymmetric, 2-D axisymmetric with swirl, 3-D flows, 3-D shell element, 2-D membrane (film casting)
- Isothermal and non-isothermal
- Steady-state, transient analysis or evolution analysis (continuation technique)
- Generalized Newtonian flow, including yield stress fluid
- Multi-modes differential viscoelastic flow (2-D and 3-D, steady-state or transient, isothermal and non-isothermal)
- Multi-modes integral viscoelastic flow (2-D) and 3-D shell, steady-state (2-D) or transient (3-D shell), isothermal and non-isothermal)
- Heat transfer including natural conduction, forced or mixed convection, conjugate (solid/fluid) heat transfer, radiation, thermal conduction in moving solids, electrical heating
- Free surfaces modeling using deforming mesh
- Inverse problem for extrusion (die lip design)
- Internal moving boundaries (interface)
- Static and dynamic contact points
- Porous media (Darcy's law)
- Chemical species mixing and reaction
- Volumetric sources of heat, mass, viscous heating, electrical potential, Joule effect, bubbling
- Fluid structure interaction (FSI)
- Simple thermo-mechanical stress analysis after cooling
- Contact detection
- Mesh superposition technique (overlapping mesh method)
- Lagrangian trajectory calculation including statistical analysis
- Conversion of system of units
- Windows®-style organizer
  - Online access to Web services
  - Files chronology tracking system
- User-defined templates
- Interface to VisualDOC® (third-party optimization software)
- Expert system giving indications about:
  - Diagnostic for non-convergence and possible remedies
  - Mass and energy conservation
  - Adding missing iterations if necessary
  - Rate of convergence
  - Immediate stop of the run if divergence occurs
  - Current memory requirement
  - Recommendation of techniques to reduce CPU time for further similar simulations
  - Recommendation of necessary modifications of case set-up to ease convergence

Mesh Capabilities

- Quadrilateral, triangular, hexahedral (brick), tetrahedral, prism (wedge), pyramid, mixed element meshes (hybrid meshes), triangular 3-D shell element, quadrilateral 3-D shell element
- P Mesh (group of 0-D, 1-D, 2-D or 3-D topological entities)
- Non-conformal (non-matching) mesh interfaces allowed
- Interpolation including constant, linear, linear discontinuous, quadratic, mini element, 2X2, 4X4
- Import of meshes from GAMBIT®, GeoMESH®, FIGEN, POLYMESH, POLYM3D, I-deas®, PATRAN®

- Dynamic, solution-based adaptation including:
  - Conformal adaption on triangular and tetrahedral meshes
  - Hanging node adaption and mesh embedding for all element types
  - Adaptive criteria based on:
    - Mold curvature
    - Free surface curvature
    - Distance to mold
    - Local variation of quantity
    - Local mesh deformation
    - Maximum size specified in user-defined box
- Automatic interpolation of solution after mesh refinement
- Mesh manipulation tools (scaling, translation, rotation, merging)
- Remeshing techniques (deforming mesh) including:
  - Efficient 2-D remeshing technique (SPINES)
  - Robust 2-D remeshing technique (Optimesh, Elastic, Lagrangian, Thompson)
  - Efficient 3-D remeshing technique (Optimesh, Streamwise)
  - Full 3-D method (Thompson, elasticity-based, Lagrangian)
  - 3-D shell Lagrangian remeshing method
- Combination of meshes from different sources into a single file (Polyfuse)
- Online mesh information box

Numerical Method

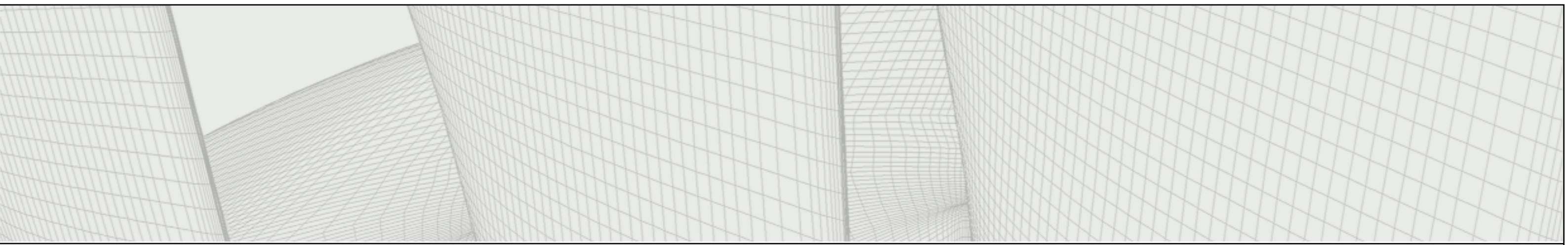
- Finite element method based on fully unstructured meshes
- Direct solver (Newton-Raphson)
- Fully coupled solver
- Option to decouple temperature and/or coordinates
- Multi-frontal solver
- Dynamic memory allocation
- Single- and double-precision calculation
- Newton-Raphson and Picard iteration scheme for viscosity
- EVSS (elastic viscous split stress) and DEVSS formulations
- Upwinding (SU), 4X4 SU
- Time integration
  - Implicit Euler
  - Implicit Galerkin
  - Crank-Nicolson

Rheological Modeling

- Generalized Newtonian laws including:
  - Newtonian (constant)
  - Bird-Carreau
  - Cross
  - Power law
  - Carreau-Yasuda
  - Bingham
  - Herschell-Bulkley
  - Log-log
  - Modified Bingham
  - Modified Herschel-Bulkley
  - Modified cross law
- Temperature dependence
  - No dependence
  - Mixed dependence (polynomial expression)
  - Arrhenius approximate (first-order)
  - Arrhenius
  - Arrhenius approximate shear stress (vertical/horizontal shift)
  - Arrhenius shear stress
  - Fulcher
  - WLF
  - WLF shear stress (vertical/horizontal shift)
- Additional dependence via UDF
  - Residence time (polymer aging)
  - Coordinates
  - Velocities
  - Strain rate
  - Invariants of rate of deformation tensors
  - Pressure
  - Temperature
  - Species
  - User-defined quantities
- Automatic fitting tool for viscometric and rheometric curves
  - Shear rate vs. shear viscosity
  - Loss and storage moduli vs. frequency
  - First and second normal difference vs. frequency
  - Elongational viscosity (constant elongation rate) vs. time
  - Stress vs. strain (constant elongation speed)
- Multi-mode viscoelastic models (differential and integral) as add-on module

Boundary Conditions

- Inlet velocity in terms of Cartesian or cylindrical-polar components, magnitude and direction, magnitude of normal-tangential components or user-specified local coordinate components
- Inlet velocity profile calculated as a pre-processor considering the volumetric flow rate, slip coefficient and rheological behavior
- Exit static pressure
- Outflow, with specified flow rate weighting
- Outflow (Vs = 0 and Fn = Cst)
- Take-up force
- Take-up velocity
- Wall boundaries, with specification of:
  - Tangential wall velocity using Cartesian component form, rotational speed or local axis
  - Shear stress including slip conditions
  - Thermal boundary conditions using heat-flux, temperature or external convection, radiation (emissivity), mixed conditions or user-specified temperature profile
  - Rosseland correction
- Moving boundaries (free surface and interface), with specification of:
  - Specified normal force
  - Specified normal velocity
  - Air drag force
  - Slipping along the interface between two fluids
  - Surface/interface tension



- Symmetry, rotationally periodic and translationally periodic boundaries
- Axis boundary conditions
- Specified normal and/or tangential force in combination with normal and tangential velocity
- Specified normal and/or tangential force in combination with normal and tangential displacement (FSI)
- Vanishing velocity along the solid (FSI)
- Partial slip along the solid (FSI)
- Imposed nodal displacement (FSI)
- Thermal interface between flowing and solid materials
- Interface between Navier-Stokes and Darcy's law
- Partial slip for laminar flow
  - Navier's law
  - Coulomb's friction (using UDF)
  - Threshold law
  - Asymptotic law
  - Arrhenius dependence with request to temperature
- Partial slip (Navier's law) along moving parts (using the mesh superposition technique)
- Contact detection
  - 2-D mechanical contact
  - 3-D mechanical contact
  - Heat transfer with the mold
  - Slip behavior along the contact wall (Navier's law)
  - FSI: stress calculation in the mold induced by parison contact
- Periodic conditions
- Transient conditions
- User-specified profile or map of boundary condition under CSV format
- User-specified profile or map of initial condition under CSV format
- Optimization of initial thickness map for blow molding applications

Material Properties

- Constant or variable fluid properties including temperature and composition dependence (data pair or piecewise polynomial input) including thermal conductivity, specific heat, density
- Constant or variable solid properties including temperature and composition dependence (data pair or piecewise polynomial input) including thermal conductivity, specific heat, density
- Use of database containing material properties for standard fluids and solids (user-modifiable)
- Temperature-dependent heat capacity and thermal conductivity in solid regions
- User-defined property inputs
- Automatic fitting tool for material properties
- Gravity
- Inertia term
- Viscous heating
- Heat source
- Temperature variation of the density (Boussinesq approximation)
- Surface tension
- Young modulus
- Poisson coefficient
- Linear dilation coefficient
- Interface to CAMPUSTM data base
- Crystallization models
  - Doufas-McHugh
  - Nakamura (via UDF)

Chemical Reaction and Combustion Modeling

- Finite rate chemistry for N reactions with backward reactions using:
  - Arrhenius
  - User-defined function
- User-defined access to reaction source/sink terms
- Physical foaming model (PE)
- Curing model

User-Defined Functions

- Definition of custom physical properties
- Customized boundary conditions and initial conditions
- Creation of custom post-processing variables

Parallel Processing

- Parallel processing on shared memory systems for SGI®, Compaq® α, Intel®, HP-UX®
- Domain decomposition method, with grid partitioning tools using METIS

Interface, Graphics, Post-processing and Reporting

- Grid checking (validity, quality, size), merging, separating and reordering
- Summary reports of solver and physical model settings
- Flexible units specification (SI units, British units, custom/mixed units)
- Reporting and monitoring of fluxes of mass, heat, chemical species
- Reporting and monitoring of forces and torques using the mesh superposition technique
- Transformation of data via pre-defined functions
- Computation and reporting of surface integrals and averages
- Computation and reporting of volume integrals and averages
- Calculator utility for user-defined field functions
- Calculation of gradients (vector and scalar) and derived quantities
- Histograms of geometric and solution data
- Quantitative XY plotting of data
- Graphical probing of data

- Statistical tool (POLYSTAT) to quantify mixing from a large number of trajectories
  - Mean and standard deviation
  - Probability function
  - Density of probability function
  - Histograms
  - Percentiles
  - Correlation between variables
  - Distributive mixing
  - Carbon black disagglomeration model
  - See also exported quantities

Data Export

- Export of solution data to:
  - FIELDVIEW™
  - I-deas®
  - PATRAN®
  - CFView
  - FIPOST
  - FLPOST
  - EnSight® (via a FIDAP Neutral file)

Exported Quantities

- Velocity
- Pressure
- Temperature
- Streamlines
- Stress
- Stress eigenvalues
- Strain
- Viscosity
- Local shear rate (color contours and statistical analysis)
- Residence time (color contours and statistical analysis)
- Die balancing evaluation
- Flow rate across user-specified boundaries
- Thickness (for shell element)
- Permeability (for shell element)
- Weight and volumes of the flashes (blow molding and thermoforming)
- Inner volume of the container (blow molding and thermoforming)
- Weight of the container (blow molding and thermoforming)
- Area stretch ratio
- Map of contact time
- Mixing index (color contours and statistical analysis)
- Total shear (statistical analysis)
- Stretching (statistical analysis)
- Instantaneous efficiency of stretching (statistical analysis)
- Time average efficiency of stretching (statistical analysis)
- Segregation scale (statistical analysis)
- Striation thickness (statistical analysis)
- Distributive mixing index (statistical analysis)
- User-defined indices (statistical analysis)
- Vorticity number
- Force, torque along user-specified boundaries (using the mesh superposition technique)
- Dissipated power
- Convected heat
- Heat/mass flux along user-specified boundaries
- Tracking of material points
- Generation of a blow molding shell model using the results of a 2-D axisym metric parison extrusion simulation

Add-on Module: Viscoelastic Models

- Multi-mode differential viscoelastic models
  - Maxwell
  - Oldroyd-B
  - White-Metzer
  - Phan Thien-Tanner
  - Giesekus
  - FENE P
  - Pom-pom
  - Leonov
  - Simplified viscoelastic model for extrusion (PFLM)
- Multi-mode integral viscoelastic models (2-D and 3-D shell):
  - Lodge-Maxwell
  - Doi-Edwards
  - KBKZ with Wagner and Papanastasiou-Scriven-Macosko damping function (reversible or irreversible)
- Temperature dependence
  - No dependence
  - Arrhenius approximate (first-order)
  - Arrhenius
  - WLF

Online Help and Documentation

- Complete hypertext-based online documentation
- User's guide including theory and application
- Tutorial guide with model-specific examples
- Online access to the User Services Center
- Online Getting Started
- Partial online help in Japanese

Supported Hardware

- POLYFLOW 3.11 is supported, in serial and parallel, on HP-UX, Linux® 32– and 64–bits and Windows® 32– and 64–bits. Contact ANSYS, Inc. for details.

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