Development of ENGINE - A 3D Computational Tool for Modeling and Simulation of Nuclear Fuels and Materials

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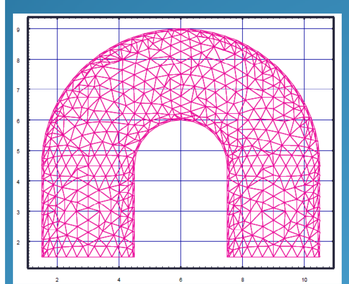
A Multi-physics simulation tool

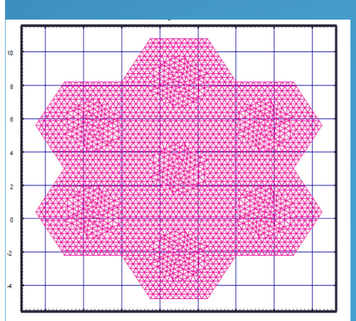
- ENGINE is equipped with advanced mathematical models based on finite element and particle based methods
- It provides a 3D platform for applying advanced physical models at various scales.
- The code consists of the following parts:
  - Material and initial/boundary condition specifications
  - Geometry specifications and 3D surface mesher
  - Material properties module
  - System discretization, gauss quadrature integration of system of equations, and matrix solver

Advantages

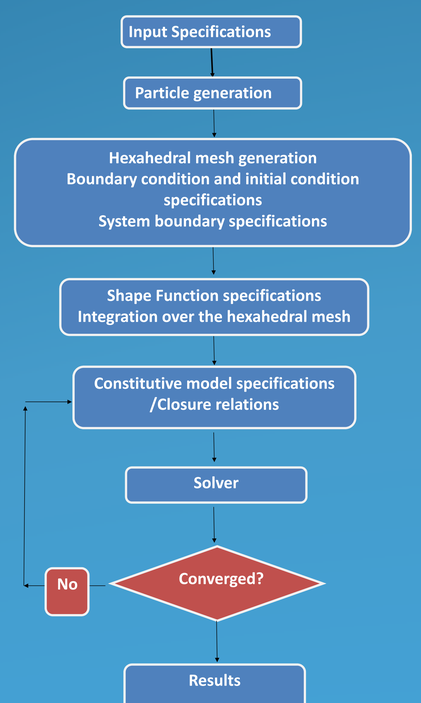
- Able to mesh complex geometries in 3D
- Fast particle generation at system boundaries via front tracking algorithm
- Fast hexahedral mesh generation over the volume.
- The hybrid algorithm largely eliminates re-meshing and advantageous in modeling moving boundary problems
- Numerical stability and able tackle with non-linearity
- The code is verified against analytical solutions for various physical phenomena

Sample Surface Meshing





Numerical Algorithm



Applications

Structural Mechanics

- Linear elasticity with incremental strain theory
- Able to simulate elastic, creep, thermal , swelling strains and residual or externally applied stress
- External stress and displacement boundary conditions are user defined
- Large deformation simulations can be performed

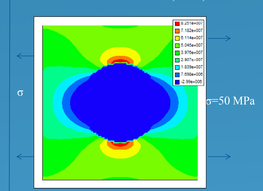
Verification Exercises

- The figure on the left shows the x-stress distribution around a void under 50 MPa applied tensile load in x direction. Stress concentration is observed near the boundary, normal to the applied stress.

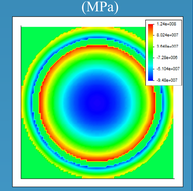
- The figure on the right shows the axial stress distribution of the fuel pin (fuel pellet and clad) under the applied temperature gradient. Stress is compressive at the inner hot regions and tensile at the outer regions for both fuel pellet and cladding.

- The predicted stress distributions are satisfactory compared with the analytical solutions for both cases.

X-stress around a void (MPa)



Fuel pin axial stress (MPa)



Heat Transfer

- Solves the steady state and time dependent heat equation
- User defined initial and boundary conditions of convective/radiative heat transfer ,constant temperature or adiabatic type

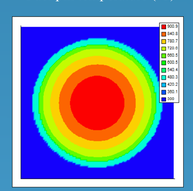
Verification Exercises

- The figure on the left shows the temperature distribution of the power producing fuel pin with the applied convective boundary condition at the clad outer surface. Coolant temperature is 300 ºC.

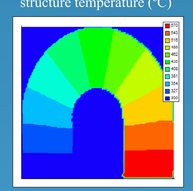
- The figure on the right shows a U-shaped support structure, convective heating at 600 ºC and cooling at 300 ºC are applied at the joint surfaces .

- The predicted temperature distributions are satisfactory compared with the analytical solutions, for both cases.

Fuel pin temperature (ºC)



U-shape support structure temperature (ºC)



Phase Transformations (Enhanced Phase Field Method)

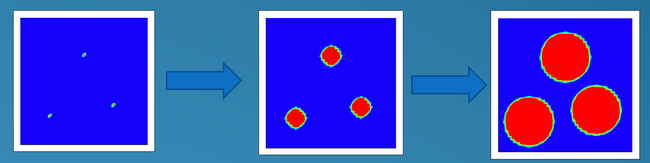
- The model solves the Cahn-Hilliard equation for the diffusing species and the Allen-Cahn equation for structural transformations.
- Free energy functional consists of chemical energy, surface energy, elastic energy, etc.
- Shape factors are used for each node in order to model the surface energy term accurately, WITHOUT requiring using a very fine mesh structure at interfaces.
- The algorithm largely eliminates re-meshing requirements.

- Sample simulations below show the nucleation and growth of the precipitates in supersaturated media.
- If the medium isotropic, spherical precipitates results as shown in the upper figures.
- A strong anisotropy in surface energy term is applied for the simulation given at the lower figures. As a result, platelet-shape precipitates grow in y-direction.

The results shows that the approach is promising and satisfactory.

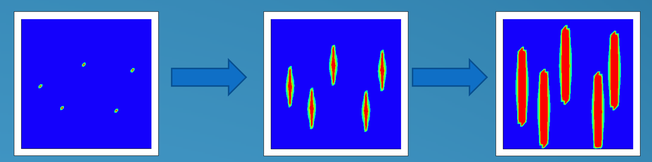
Precipitation in isotropic medium

Nucleation | 100 time steps | 250 time steps



Precipitation in a strongly anisotropic medium

Nucleation | 200 time steps | 420 time steps



Crack Propagation (Enhanced Phase Field Method)

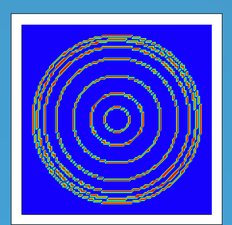
- The model solves Allen-Cahn equation to predict the crack growth behavior.
- Slip orientation and its local variation, initial crack geometry and external stress are user defined.
- Free energy functional includes elastic, surface energy, and double well potential. Plastic energy term can also be added.
- Solution of Allen-Cahn equation simulates the crack propagation towards the direction of minimum energy.

- The model is applied for a brittle material under the applied vertical tensile stress as given below. Crack tends to propagate normal to the applied stress and on the favorable slip bands. The crack growth rate rapidly increases with increased crack size as expected.

The beginning of the simulation | 100 time steps | 229 time steps

Line Dislocation Dynamics

- The model solves the equation of motion to predict the movement of the dislocations. Viscous drag and driving force terms are included.
- Dislocations are divided into lines and each line is represented via a pair of nodes. Finite element integration is performed over the line segments.
- Dislocations are allowed to glide on their slip planes only under the applied shear stress.

- The simulation result given in the figure below shows the formation and the glide of the dislocation loops via Frank-Read sources. The barrier applied to the outer surface tends to limit the outward dislocation motion and dislocation pile-up occurs near the barrier.

- The results are consistent with experimental observations.