Name: auxi
Description: auxi is a toolkit to help metallurgical process engineers with their day-to-day tasks. Many of the calculations that we do require things like molar masses, conversion of one compound to another using stoichiometry, enthalpy calculations, heat transfer calculations, mass balances, energy balances, etc. It is usually quite time consuming to get started with these calculations in a tool like Excel. auxi aims to save you time by making many of these calculations available from within Python.
url: https://github.com/Ex-Mente/auxi.0

Name: DAMASK
Description: At the core of DAMASK is a flexible and hierarchically structured model of material point behavior for the solution of elastoplastic boundary value problems along with damage and thermal physics. Its main purpose is the simulation of crystal plasticity within a finite-strain continuum mechanical framework.
url: https://damask.mpie.de/Home/WebHome

Name: Elmer
Description: Elmer includes physical models of fluid dynamics, structural mechanics, electromagnetics, heat transfer and acoustics, for example. These are described by partial differential equations which Elmer solves by the Finite Element Method (FEM).
url: https://www.csc.fi/web/elmer/elmer

Name: DREAM.3D
Description: DREAM.3D consists of data analysis tools (Filters) that allow for the construction of customized workflows (Pipelines) to analyze data. DREAM.3D provides a flexible and extensible data structure that eases data transport between collaborators by storing data in a non-proprietary format.
DREAM.3D makes the reconstruction of 3D data simple and straight forward. The development of additional features is ongoing and the DREAM.3D development team welcomes your feedback whether you are a first-time user or seasoned user.
url: http://dream3d.bluequartz.net/

Name: OpenMD
Description: OpenMD is an open source molecular dynamics engine which is capable of efficiently simulating liquids, proteins, nanoparticles, interfaces, and other complex systems using atom types with orientational degrees of freedom (e.g. “sticky” atoms, point dipoles, and coarse-grained assemblies). Proteins, zeolites, lipids, transition metals (bulk, flat interfaces, and nanoparticles) have all been simulated using force fields included with the code. OpenMD works on parallel computers using the Message Passing Interface (MPI), and comes with a number of analysis and utility programs that are easy to use and modify. An OpenMD simulation is specified using a very simple meta-data language that is easy to learn.
url: http://openmd.org/

Name: pycalphad

Description: pycalphad is a free and open-source Python library for designing thermodynamic models, calculating phase diagrams and investigating phase equilibria within the CALPHAD method. It provides routines for reading Thermo-Calc TDB files and for solving the multi-component, multi-phase Gibbs energy minimization problem.
url: https://pycalphad.org/docs/latest/

Name: ESPEI
Description: ESPEI, or Extensible Self-optimizing Phase Equilibria Infrastructure, is a tool for automated thermodynamic database development within the CALPHAD method. It uses pycalphad for calculating Gibbs free energies of thermodynamic models.
url: http://espei.org/en/latest/

Name: MatCalc
Description: MatCalc is a scientific software toolbox for computer simulation of:
constrained and unconstrained phase equilibria
multi-component and multi-phase precipitation kinetics
efficient single-class microstructure evolution of grain growth, recovery and static recrystallization
multi-class static and dynamic recrystallization with full coupling to precipitation kinetics
state parameter-based stress-strain curve
1D and 2D long-range diffusion simulation
simultaneous long-range diffusion and precipitation
phase transformations / moving phase boundaries (in development)
lattice Metropolis and kinetic Monte Carlo
url: https://www.matcalc.at/

Name: ABINIT
Description: ABINIT is a software suite to calculate the optical, mechanical, vibrational, and other observable properties of materials. Starting from the quantum equations of density functional theory, you can build up to advanced applications with perturbation theories based on DFT, and many-body Green's functions (GW and DMFT).
ABINIT can calculate molecules, nanostructures and solids with any chemical composition, and comes with several complete and robust tables of atomic potentials.
url: https://www.abinit.org/

Name: ATAT
Description: ATAT is a generic name that refers to a collection of alloy theory tools developed by Axel van de Walle, in collaboration with various research groups and with various sources of financial support.
url: https://www.brown.edu/Departments/Engineering/Labs/avdw/atat/

Name: Code_Aster
Description: Code_Aster is a large finite element code which Electricité de France (EDF) has written to solve complex problems in nuclear power. It comes with tools for adaptive

remeshing, and is ISO 9001 certified.
url: https://code-aster.org/spip.php?rubrique2

Name: CalculiX
Description: CalculiX is an implicit code for quickly calculating mechanical or thermal steady state solutions, or performing buckling calculations, but without adaptive remeshing.
url: http://www.calculix.de/

Name: OpenFOAM
Description: OpenFOAM comes from the OpenCFD Ltd. consulting company, and includes an extensive set of solvers, utilities for pre-and post-processing, and physical model toolbox libraries. It runs in parallel with an efficient iterative implicit time-stepping scheme, and includes several turbulence models
url: https://openfoam.org/

Name: LibMesh
Description: LibMesh is a parallel finite element library with implicit time stepping, adaptive remeshing, and dynamic repartitioning across a cluster. Like FiPy, it can solve fourth-order biharmonic equations needed for Cahn–Hilliard phase field simulations. Unfortunately, it has no user interface at all; to generate a new simulation, one must write a short C++ program which calls the library's functions.
url: https://libmesh.github.io/

Name: CODE_SATURNE
Description: Code_ Saturne is the EDF fluid dynamics counterpart to Code_Aster, and features magneto-hydrodynamics, incompressible or compressible flows, multi-phase flows (arbitrary Lagrange–Euler mesh deformation), and turbulence models, along with advanced heat transfer capabilities such as radiation and combustion.
url: https://www.code-saturne.org/cms/

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