Introduction

In this documentation we will provide instructions on how to access RGTFun, an example calculation using RGTFun that can be used as a tutorial for new users, and then discuss the included testing suite. Documentation for all functions can be found in the appendix.

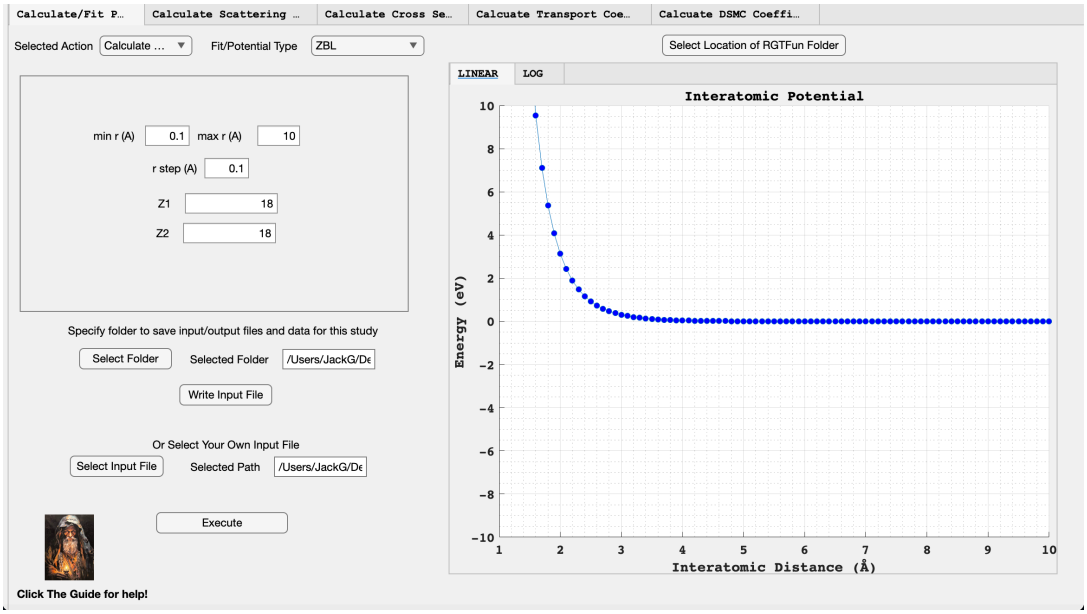
Accessing RGTFun

RGTFun can be downloaded from the public Github repository linked here:
https://github.com/nbb2/rgtfun/tree/paper
Please download all folders from the repository and ensure that they are all located within a *RGTFun* folder on your machine (it does not have to be called *RGTFun*). This is important because the app will ask you to select the RGTFun folder on your machine so it can establish the path to the *src* and *gui* folders. It does not matter where your *RGTFun* folder is located as long as it is a local folder, i.e. not in a cloud service. Once downloading the repository folders, you can start the app by opening the *gui.mlapp* file in the *gui* folder.

An Example Calculation of Argon-Argon Interaction

We will now present example calculations of transport quanitities and scattering integrals using RGTFun. The calculations will be performed for an Argon-Argon ZBL potential.

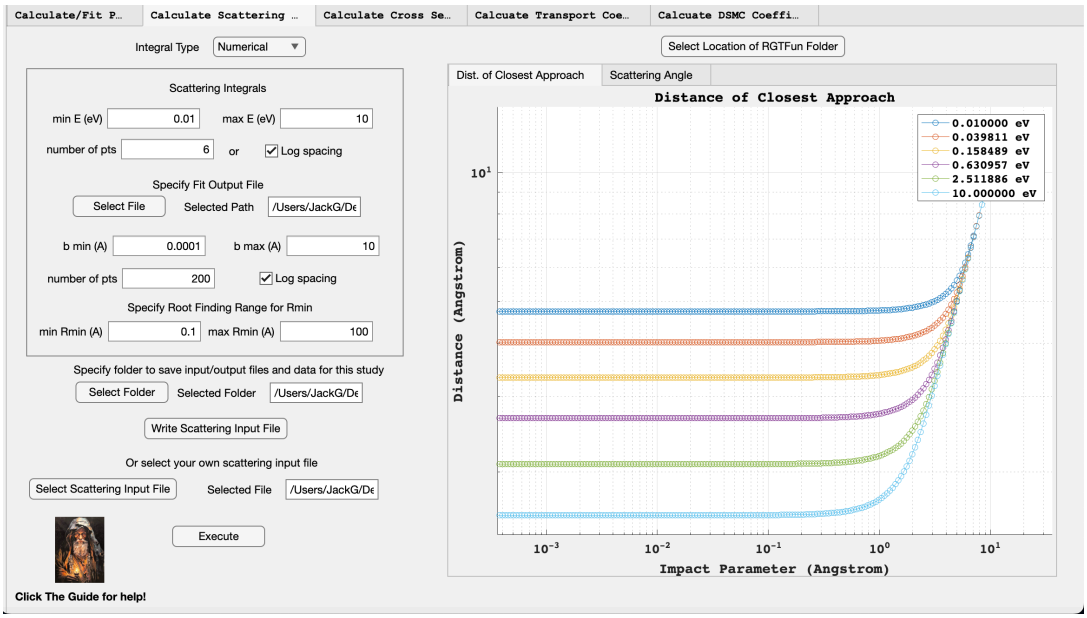
Calculate/Fit Potential Tab



Screenshot of *Calculate/Fit Potential* tab for an Argon-Argon ZBL potential.

The *Calculate/Fit Potential* tab allows you to either create your own potential data or fit one of the RGTFun-supported potentials to your own data. For this example, we wanted to calculate a ZBL potential for an Argon-Argon interaction. To begin, we selected “Calculate Potential” from the “Selected Action” drop-down menu. Then, we selected “ZBL” from the “Fit/Potential Type” drop-down menu. We then specified the distance values and potential parameters. Then we selected the folder where RGTFun will save the input/output files and data. We then clicked “Write Input File” to generate an input file with the potential parameters specified. This will auto populate the “Or Select Your Own Input File” box. Lastly, we selected “Execute” to generate potential data, plot the potential data, save the plot as an image, and save a fit output file for the data.

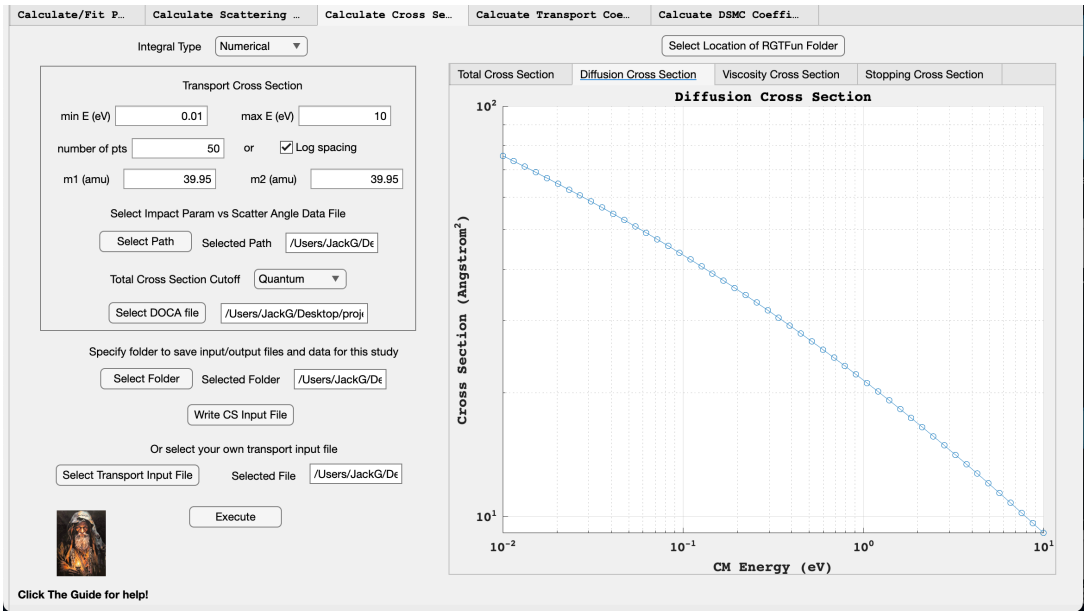
Calculate Scattering Integrals Tab



Screenshot of *Calculate Scattering Intergrals* tab for an Argon-Argon ZBL potential.

The *Calculate Scattering Integrals* tab allows you to calculate the distance of closest approach (DOCA) and scattering angle as a function of impact parameter. First, we chose “Numerical” from the “Integral Type” drop down menu becuase we wanted to use our potential data from the previous tab. We then specified the energy range for calculating the quantities. Since we wanted log spacing for the energy values, we clicked the “Log spacing” box and specifed the number of points. Note that our fit output file was autopopulated after we clicked “Execute” in the previous tab. We then specified the impact parameter range to integrate over and chose to use log spacing for these values. We then specified a range for the root solver used in the DOCA calculations. We then clicked “Write Scattering Input File” to write the input file and clicked “Execute” to generate datasets for the DOCA and scattering angle, save those data sets to our “study” folder, and save the figures as images.

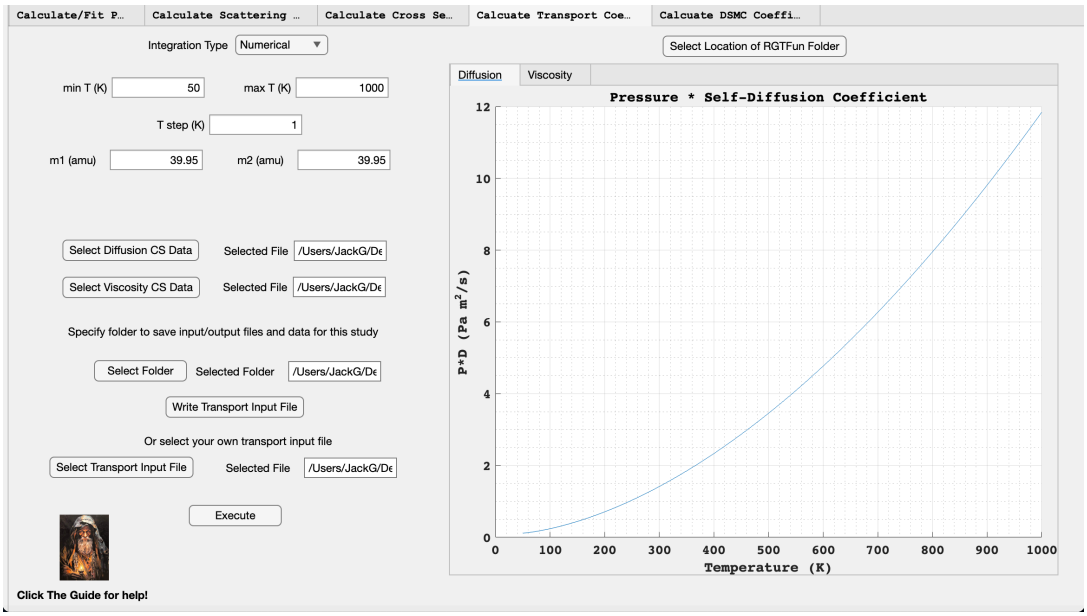
Calculate Cross Sections Tab



Screenshot of *Calculate Cross Sections* tab for an Argon-Argon ZBL potential.

The *Calculate Cross Sections* tab allows you to calculate total cross section, diffusion cross section, viscosity cross section, and stopping cross section. First, we selected “Numerical” from the “Integral Type” drop-down, which will use the scattering angle vs. impact parameter data from the previous tab. While the energy values from the previous tab autopopulate into this tab, we have increased the number of energy points from what was used in figure 7 to reduce error in the trapezoidal integrals used in this tab. We then specified the atomic mass of Argon in atomic units. Note that the file path of the scattering angle data was autopopulated when the previous tab was executed. Then we chose to use a quantum mechanical cutoff for the total cross section. Then, we clicked “Write CS Input File” to create the input file for the cross section calculations. Lastly, we clicked “Execute” to calculate the cross sections, save the data as csv files in our “study folder”, and save the figures as images.

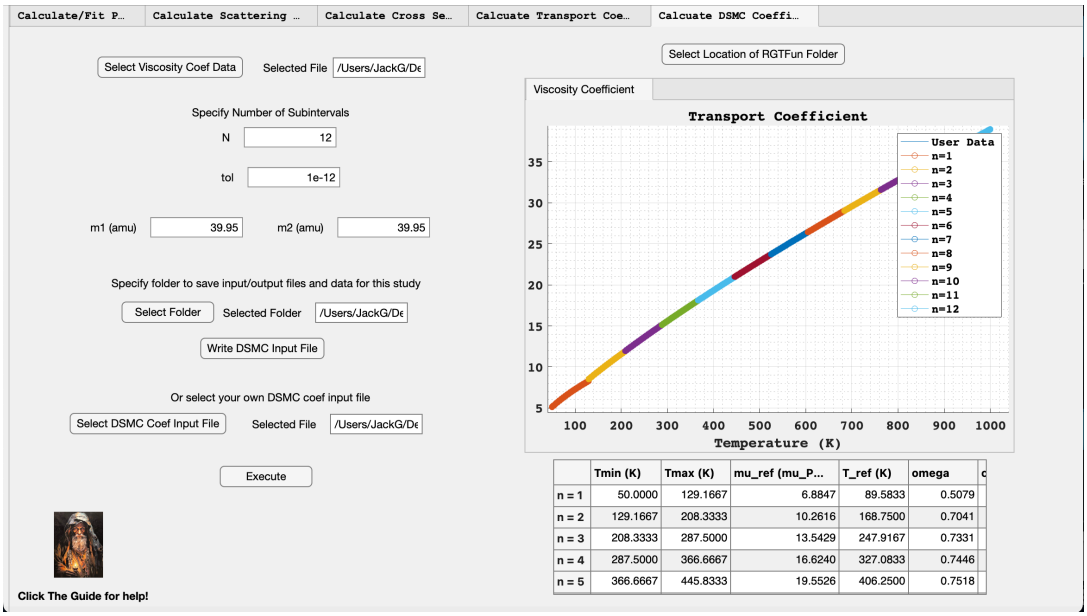
Calculate Transport Coefficients Tab



Screenshot of *Calculate Transport Coefficients* tab for an Argon-Argon ZBL potential.

The tab allows you to calculate the self-diffusion coefficient and viscosity coefficient for user-specified temperatures. First, we selected “Numerical” from the “Integration Type” drop down, which allows us to use the cross section data from the previous tab. Next, we specified the temperature range (in Kelvin) that the code should use to calculate the transport coefficient data. Note that the atomic masses of the present species, as well as the locations of the cross section data files, were autopopulated from the previous tab. We then clicked “Write Transport Input File” to write the input file to our “study” folder. Lastly, we clicked “Execute” to calculate the self-diffusion and viscosity coefficient data, save the data as csv files in our “study” folder, plot the data, and save the plots as images.

Calculate DSMC Coefficients Tab



Screenshot of *Calculate DSMC Coefficients* tab for an Argon-Argon ZBL potential.

The *Calculate DSMC Coefficients* tab allows the user to calculate the ω parameter for the VHS DSMC model. This parameter is calculated by fitting the VHS diffusion coefficient expression to the user-provided viscosity coefficient data. Note that the location of our viscosity coefficient data file was autopopulated upon execution of the previous tab. Next, we specifed the number of subintervals to split the data into for fitting. An ω parameter will be calculated for each subinterval. We also specifed the tolerance for the fitting. A tolerance of 1e-12 or lower is suggested. Note that the atomic masses of the present species were autopopulated from the previous tab. We then clicked “Write DSMC Input File” to write the input file to our “study folder”. Lastly, we clicked “Execute” to calculate an ω parameter for each subinterval of our viscosity coefficient data, as well as a collision diameter for each subinterval. Our viscosity coefficient data from the previous tab and the fitted subintervals are plotted. All relevant quantities are visible in the tab’s table. This table is saved to our “study” folder.

RGTFun Test Suite

A test suite has been included in the main RGTFun distribution so that users can verify their version is functioning correctly. Test functions were written to verify the functionality of all main functions within RGTFun. The test functions are located in the *test* folder within the main *RGTFun* folder. All test reference data is located in the *testFiles* folder. To run the tests, please change directories to the *test* folder and load the test functions in the MATLAB Test Browser. Then run the current suite, and verify that all tests were executed successfully.

Appendix:Function Documentation

Table of Contents

DOCAroot

```
function r0 = DOCAroot(Ec,b,V,rmin,rmax,chebfunpath)
%DOCAROOT    Outputs float value for the root of the DOCA equation.
%   Y=DOCAROOT(EC,B,V,RMIN,RMAX) generates a float value for the root
%   of the distance of closest approach (DOCA) equation using two
%   iterations of the CHEBFUN root finding package.
%
%   -- EC must be the the energy in eV.
%   -- B must be the impact paramter in Angstrom.
%   -- V must be the potential function handle.
%   -- RMIN is the lower bound of possible root values in Angstrom.
%   -- RMAX is the upper bound of possble root values in Angstrom.
%
%   See also GMQUADSCATTERINGANGLE RUN_SCATTERINGINTEGRALS
    addpath(chebfunpath)
    chebDOCA = chebfun(@(r) doca(r,Ec,b,V),[rmin,rmax]);
    ri = max(roots(chebDOCA));
    chebDOCA2 = chebfun(@(r) doca(r,Ec,b,V),[0.9*ri,1.1*ri]);
    r0 = max(roots(chebDOCA2));

end

function d = doca(r,Ec,b,V)
%MY_DOCA Ouputs the DOCA equation.
%   Y=MY_DOCA(R,EC,B,V) generates the DOCA equation.
%   -- R is a placeholder value for distance.
%   -- EC must be the energy in eV.
%   -- B must be the impact parameter in Angstrom.
%   -- V is the potential function handle.
%
%   See also DOCAROOT
    d = r^2 - ((r^2)*V(r)/Ec) - (b^2);
end
```

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GMquadScatteringAngle

```
function th = GMquadScatteringAngle(V,Ec,b,rm,n)
%GMQUADSCATTERINGANGLE    Outputs float scattering angle.
%   Y=GMQUADSCATTERINGANGLE(V,EC,B,RM,N) generates a float value for the
%   scattering angle using GM Quadrature.
%
%   -- V must be the potential function handle.
%   -- EC must be the the energy in eV.
%   -- B must be the impact paramter in Angstrom.
%   -- RM is the distance of closest approach in Angstrom.
%   -- N is the number of trapezoids to use.
%
%   See also DOCAROOT RUN_SCATTERINGINTEGRALS
    sum = 0;
    for j = 1:(n/2)
        anj = cos(((2*((n/2) - j + 1) - 1)/(2*n))*pi);
        aj = cos(((2*j - 1)/(2*n))*pi);
        gj = (   1 - (V(rm/aj)/Ec) - ((b^2 * aj^2)/(rm^2)))^(-1/2);
        sum = sum + (anj * gj);
    end
```

```
    th = pi * (1 - ((2*b*sum)/(n*rm)));
end
```

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VHScoef

```
function y = VHScoef(fitT,T_sample,mu_sample,excludeT,vq,tol)
%VHSCOEF  Outputs sample visc value and VHS param.
%   Y=VHSCOEF(FITT,T_SAMPLE,EXCLUDET,VQ,TOL) outputs a reference
%   viscosity value and VHS parameter omega by fitting the VHS model to
%   user-specified visocity coefficient data.
%
%   -- FITT must be the interpolated temperature values in K.
%   -- T_SAMPLE must be the reference temperature value.
%   -- EXCLUDET must be a logical array of what temp values to use.
%   -- VQ must be the interpolated viscosity coefficient values with the
%   same dimension as FITT.
%   -- TOL must be the fitting tolerance.
%
%   See also RUN_DSMCCOEF
fitcoef = vq;
fitcoef(excludeT) = [];
fitchar = sprintf("(%f)*(T/(%f)).^(a)",mu_sample,T_sample);
ft = fittype(fitchar,dependent="y",...
        independent="T",coefficients="a");
coeffit = fit(fitT',fitcoef',ft,'TolFun',tol);
omega = coeffvalues(coeffit);
y = [mu_sample,omega];
end
```

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VHSviscosity

```
function y = VHSviscosity(T,omega,T_ref,mu_ref)
%VHSVISCOSITY  Outputs float array with viscosity coefficient values.
%   Y=VHSVISCOSITY(T,OMEGA,T_REF,MU_REF) generates a float array
%   containing viscosity coefficient value for each value of T using the
%   VHS model.
%
%   -- T must be a float array of temperature values in K.
%   -- OMEGA must be the VHS parameter.
%   -- T_REF must be the reference temp in K.
%   -- MU_REF must be the reference viscosity value.
%
%   See also RUN_DSMCCOEF
y = mu_ref*(T/T_ref).^omega;
end
```

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VSSalpha

```
function y = VSSalpha(omegavals,m,molar,Tvals,difvals,diams)
%VSSALPHA  Outputs VSS param alpha.
%   Y=VSSALPHA(OMEGAVALS,M,MOLAR,TVALS,DIFVALS,DIAMS) outputs VSS parameter
%   alpha using reference diffusion coefficient and collision diameter data.
%
%   -- OMEGAVALS must be an array of reference omega values.
%   -- M must be the mass of a particle in kg.
%   -- MOLAR must be the molar mass in kg.
%   -- TVALS must be an array of the reference temperature values in K.
%   -- DIFVALS must be an array of the reference diffusion coefficient data.
%   -- DIAMS must be an array of the reference collision diameteres in angstrom.
%
%   See also RUN_VSSCOEF
kb = 1.380649E-23; %J/K
Na = 6.022E23;
rhoD = molar*difvals./(Na*kb*Tvals);
y = ((4*(5-2*omegavals).*rhoD.*(diams.^2))./(3*sqrt(m*kb*Tvals/pi))) - 1;
end
```

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VSScoef

```
function y = VSScoef(minT,maxT,Tfine,vq,m,omega,P,tol)
%VSSCOEF  Outputs VSS params alpha and d.
%   Y=VSSCOEF(MINT,MAXT,TFINE,VQ,M,OMEGA,P,TOL) outputs VSS parameters
%   alpha and d by fitting the VSS model to user-specified diffusin
%   coefficient data.
%
%   -- MINT must be the lower bound of the temp range in K.
%   -- MAXT mut be the upper bound of the temp range in K.
%   -- TFINE must be the interpolated temperature values in K.
%   -- VQ must be the interpolated diffusion coefficient values with the
%   same dimension as TFINE.
%   -- M must be the reduced mass of the system in amu.
%   -- OMEGA must be the VHS param.
%   -- TOL must be the fitting tolerance.
%
%   See also RUN_DSMCCOEF
kb = 8.617333262E-5; %eV/K
excludeT = ((Tfine < minT) | (Tfine > maxT));
fitcoef = vq;
fitT = Tfine;
fitT(excludeT) = [];
fitcoef(excludeT) = [];
T_sample = 0.5*(minT + maxT);
cref = 2*(2.5-omega)*kb*T_sample/m;
fitchar = sprintf("157377.3718*30000*(a+1)*(pi^0.5)*((%e)*T).*((pi*2*(%e)*T/(%e)).^(%e))/(16*a*gamma(3.5-%e)*(%e)*pi*(d^2)*(%e)
    kb,kb,m,omega,omega,P,cref,omega);
ft = fittype(fitchar,dependent="y",...
        independent="T",coefficients=["a" "d"]);
coeffit = fit(fitT',fitcoef',ft,'TolFun',tol,'Lower',[0 0],...
                    'Upper',[10 10],'StartPoint',[1 1]);
coefs = coeffvalues(coeffit);
alpha = coefs(1);
```

```
d = coefs(2);
y = [alpha,d];
end
```

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VSSconvergence

```
function y = VSSconvergence(alphavals,omegavals,m,Tvals,difvals,muref,tol)
%VSSCONVERGENCE  Checks least squares convergence of VSS parameters.
%   Y=VSSCONVERGENCE(ALPHAVALS,OMEGAVALS,M,TVALS,DIFVALS,MUREF,TOL) outputs
%   TRUE or FALSE depending on if the user-specified least-squares
%   tolerance is satisfied.
%
%   -- ALPHAVALS must be an array of the alpha values at each reference temperature.
%   -- OMEGAVALS must be an array of the omega values at each reference
%   temperature.
%   -- M must be the mass of a particle in kg.
%   -- TVALS must be an array of the reference temperature values in K.
%   -- DIFVALS must be an array of the reference diffusion coefficient data.
%   -- MUREF must be an array of the reference viscosity coefficient data.
%   -- TOL must be the user-specified least squares tolerance.
%   See also RUN_VSSCOEF
kb = 1.380649E-23; %J/K
Na = 6.022E23;
rhoD = m*difvals./(Na*kb*Tvals);
muvals = ((10./alphavals)+5).*rhoD./(21-6*omegavals);
Sc = rhoD./muref; %Schmidt number
LSerror = sum((muvals - muref).^2);
y = (LSerror > tol);
end
```

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VSSdiameter

```
function y = VSSdiameter(alphavals,omegavals,m,Tvals,muvals)
%VSSDIAMETER  Outputs VSS collision diameter.
%   Y=VSSDIAMETER(ALPHAVALS,OMEGAVALS,M,TVALS,MUVALS) outputs VSS collision
%   diamater using reference viscosity coefficient and VHS parameter data.
%
%   -- ALPHAVALS must be an array of the alpha values at each reference temperature.
%   -- OMEGAVALS must be an array of reference omega values.
%   -- M must be the mass of a particle in kg.
%   -- TVALS must be an array of the reference temperature values in K.
%   -- MUVALS must be an array of the reference viscosity coefficient data.
%
%   See also RUN_VSSCOEF
kb = 1.380649E-23; %J/K
y2 = ((5*(alphavals+1).*(alphavals+2).*sqrt(m*kb*Tvals/pi))./...
    (4*alphavals.*(5-2*omegavals).*(7-2*omegavals).*muvals)); % meters
y = sqrt(y2);
end
```

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VSSdiffusion

```
function y = VSSdiffusion(T,omega,a,d,m,P,T_sample)
%MY_VSSDIFFUSION  Outputs float array with diffusion coefficient values.
%   Y=MY_VSSDIFFUSION(T,OMEGA,A,D,M,P,T_SAMPLE) generates a float array
%   containing diffusion coefficient value for each value of T using the
%   VSS model.
%
%   -- T must be a float array of temperature values in K.
%   -- OMEGA must be the VHS parameter.
%   -- A must be the alpha VSS parameter.
%   -- D must be the d VSS parameter.
%   -- M must be the reduced mass in amu.
%   -- P must be the pressure in bar.
%   -- T_SAMPLE must be the reference temp in K.
%
%   See also RUN_DSMCCOEF
%kb = 1.380649E-23; %J/K
kb = 8.617333262E-5; %eV/K
cref = 2*(2.5-omega)*kb*T_sample/m;
fprintf('cref is %f\n',cref)
y = 157377.3718*30000*(a+1)*(pi^0.5)*(kb*T).*((pi*2*kb*T/m).^omega)/(16*a*gamma(3.5-omega)*...
    P*pi*(d^2)*(cref)^(omega - 0.5));
end
```

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coulomb

```
function y = coulombchar(z1)
%COULOMBCHAR    Outputs character array with fitting model.
%   Y=COULOMBCHAR(Z1) generates a char array containing
%   the Coulomb potential equation with the user-specified Z1.
%
%   -- Z1 must be the integer atomic number of species 1.
%
%   See also RUN_FITPOTENTIAL
    eps_naught = 0.005526349406; %e^2 * eV^-1 * Angstrom^-1
    Ke = 1/(4*pi*eps_naught);
    y = sprintf("(%d)*%i*z2./x",Ke,z1);
end
```

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coulombchar

```
function y = coulombchar(z1)
%COULOMBCHAR    Outputs character array with fitting model.
%   Y=COULOMBCHAR(Z1) generates a char array containing
%   the Coulomb potential equation with the user-specified Z1.
%
%   -- Z1 must be the integer atomic number of species 1.
%
%   See also RUN_FITPOTENTIAL
    eps_naught = 0.005526349406; %e^2 * eV^-1 * Angstrom^-1
    Ke = 1/(4*pi*eps_naught);
    y = sprintf("(%d)*%i*z2./x",Ke,z1);
end
```

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---

diffusion_coef

```
function y = diffusion_coef(well_depth,T,m1,m2,d,inttype,data)
%DIFFUSION_COEF    Outputs self-diffusion coefficient.
%   Y=DIFFUSION_COEF(WELL_DEPTH,T,P,M1,M2,D,INTTYPE,DATA) generates a float
%   array containing a self-diffusion coefficient value for each temperature
%   using a Lennard_Jones potential (from "Khrapak, S.A. Accurate transport
%   cross sections for the Lennard-Jones potential. Eur. Phys. J. D 68, 276
%   (2014)"). Units of self-diffusion coefficient are cm^2 /s.
%
%   -- WELL-DEPTH must be the LJ well-depth in Kelvin.
%   -- T must be a float array containing temperature values in units of K.
%   -- P must be the pressure in bar.
%   -- M1 must be the mass of species 1 in amu.
%   -- M2 must be the mass of species 2 in amu.
%   -- D must be the sigma LJ parameter in units of Angstrom.
%   -- INTTYPE must be a character string specifying if the integral will
%   be exact or numerical.
%   -- DATA must be a character string filepath that gives the location of
%   the cross section data.
%
%   See also RUN_TRANSPORTCS
Tjoul = T.*(1.380649e-23);
mu = (m1*m2)/(m1+m2);
mukg = mu*(1.66054e-27);
dm = d*(1e-10);
Tstar = T/well_depth;
if strcmp(inttype,'Exact LJ')
    y = (3*sqrt(2*pi)/16)*((Tjoul).^(3/2))./(((mukg)^(1/2))* ...
    ((dm)^2)*reduceddifint(Tstar)); %PD in units of Pa * m^2 / s
elseif strcmp(inttype,'Trapezoidal LJ')
    y = (3*sqrt(2*pi)/16)*((Tjoul).^(3/2))./(((mukg)^(1/2))* ...
    ((dm)^2)*reduceddifquad(Tstar,data)); %PD in units of Pa * m^2 / s
else
    disp('Invalid Integration Type. Please check input file and try again.')
end
end

function y = reduceddifint(Tstar)
%REDUCEDDIFINT    Outputs the reduced diffusion integral.
%   Y=REDUCEDDIFINT(TSTAR) generates a float array containing a value
%   for the exact reduced diffusion integral in Khrapak, S.A. Accurate transport
```

```
%   cross sections for the Lennard-Jones potential (2014).
%
%   -- TSTAR is  float array containing the reduced temperature values.
y = zeros(size(Tstar));
ct = 1;
for t = Tstar
reddifintegrand = @(x) 0.5*(x.^2).*exp(-x).*diffusioncs(1./(2*t*x));
y(ct) = integral(reddifintegrand,0,Inf);
ct = ct + 1;
end
end

function y = reduceddifquad(Tstar,data)
%REDUCEDDIFQUAD    Outputs the reduced diffusion integral using quadrature.
%   Y=REDUCEDDIFQUAD(TSTAR,DATA) generates a float array containing a value
%   for the reduced diffusion integral in Khrapak, S.A. Accurate transport
%   cross sections for the Lennard-Jones potential (2014) using trapezoidal
%   integration.
%
%   -- TSTAR is  float array containing the reduced temperature values.
%   -- DATA is a char array containing the filepath of the cross-section
%   data.
y = zeros(size(Tstar));
ct = 1;
csdata = readmatrix(data);
for t = Tstar
X = 1./(2*t*csdata(:,1));
reddifintegrand = -0.25*(X.^2).*exp(-X).*csdata(:,2)./(t*csdata(:,1).^2);
y(ct) = trapz(csdata(:,1),reddifintegrand);
ct = ct + 1;
end
end
```

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---

diffusioncs

```
function y = diffusioncs(beta)
%DIFFUSIONCS    Outputs float array with diffusion cross-section values.
%   Y=DIFFUSIONCS(BETA) generates a float array containing diffusion
%   cros-section value for each value of the scattering parameter beta
%   using a Lennard_Jones potential.
%
%   -- BETA must be a float array containing values for the dimensionless
%   scattering parameter.
%
%   See also VISCOSITYCS RUN_TRANSPORTCS
fLEd = 1 - 0.019.*(beta.^(-1)) + 0.038.*(beta.^(-2)) - 0.049.*(beta.^(-3)) ...
    + 0.015.*(beta.^(-4));
fHEd = 1 - 0.692.*(beta) + 9.594.*(beta.^(2)) - 8.284.*(beta.^(3)) ...
    - 2.355.*(beta.^(4));

y = zeros(size(beta));
%%Case 1: beta < 0.506
idx1 = beta < 0.506;
y(idx1) = 4.507.*(beta(idx1).^(1/6)).*fHEd(idx1);

%%Case 2: beta > 0.506
```

```
idx2 = beta > 0.506;
y(idx2) = 9.866.*(beta(idx2).^(1/3)).*fLEd(idx2);
end
```

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difscatter

```
function y = difscatter(z1,z2,theta,E)
%DIFSCATTER    Outputs differential scattering cross section.
%   Y=DIFSCATTER(Z1,Z2,THETA,E) generates a float array containing
%   a differential scattering cross section value for each scattering
%   angle using the Rutherford scattering model. Units of differential
%   scattering cross section are Angstrom^2 / sr.
%
%   -- Z1 must be the integer atomic number of species 1.
%   -- Z2 must be the integer atomic number of species 2.
%   -- THETA must be the float array containing scattering angle values in
%   units of radians.
%   -- E must be the incident energy as numeric char in units of eV.
%
%   See also RUN_SCATTERINGINTEGRALS
    eps_naught = 0.005526349406; %e^2 * eV^-1 * Angstrom^-1
    Ke = 4*pi*eps_naught;
    y = (z1*z2./(4*Ke*E.*sin(theta/2).^2)).^2;
end
```

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distclose

```
function y = distclose(z1,z2,b,E)
%DISTCLOSE    Outputs distance of closest approach.
%   Y=DISTCLOSE(Z1,Z2,B,E) generates a float array containing an
%   impact parameter value for each scattering angle using the
%   Rutherford scattering model. Units of distance of closest approach
%   are Angstroms.
%
%   -- Z1 must be the integer atomic number of species 1.
%   -- Z2 must be the integer atomic number of species 2.
%   -- B must be the float array containing impact parameter values in
%   units of Angstroms.
%   -- E must be the incident energy as numeric char in units of eV.
%
%   See also RUN_SCATTERINGINTEGRALS
    eps_naught = 0.005526349406; %e^2 * eV^-1 * Angstrom^-1
    Ke = 1/(4*pi*eps_naught);
    gamma = (Ke*z1*z2/E);
    y = 0.5*(gamma+sqrt(gamma^2 + 4*(b.^2)));
end
```

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impact

```
function y = impact(z1,z2,theta,E)
%IMPACT    Outputs impact parameter.
%   Y=IMPACT(Z1,Z2,THETA,E) generates a float array containing an
%   impact parameter value for each scattering angle using the
%   Rutherford scattering model. Units of impact parameter are Angstrom.
%
%   -- Z1 must be the integer atomic number of species 1.
%   -- Z2 must be the integer atomic number of species 2.
%   -- THETA must be the float array containing scattering angle values in
%   units of radians.
%   -- E must be the incident energy as numeric char in units of eV.
%
%   See also RUN_SCATTERINGINTEGRALS
    eps_naught = 0.005526349406; %e^2 * eV^-1 * Angstrom^-1
    Ke = 4*pi*eps_naught;
    y = z1*z2.*cot(theta/2)./(2*Ke*E);
end
```

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lj_124

```
function y = lj_124(eps_well,sig,r)
%LJ_124    Outputs Lennard Jones potential data.
%   Y=LJ_124(EPS_WELL,SIG,R) generates a float array containing
%   a potential energy value for each r value using the 12-4 Lennard Jones
%   potential. Units of potential energy are eV.
%
%   -- EPS_WELL must be the float LJ well depth.
%   -- SIGMA must be the float distance at which the potential is zero.
%   -- R must be the numerical array containing r values in units of
%   Angstrom.
%
%   See also RUN_CALCPOTENTIAL
    y = (0.5)*(3^1.5)*eps_well*(((sig./r).^12)-((sig./r).^4));
end
```

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lj_126

```
function y = lj_126(eps_well,sig,r)
%LJ_126    Outputs Lennard Jones potential data.
%   Y=LJ_126(EPS_WELL,SIG,R) generates a float array containing
%   a potential energy value for each r value using the 12-6 Lennard Jones
%   potential. Units of potential energy are eV.
%
%   -- EPS_WELL must be the float LJ well depth.
%   -- SIGMA must be the float distance at which the potential is zero.
%   -- R must be the numerical array containing r values in units of
%   Angstrom.
```

```
%
%   See also RUN_CALCPOTENTIAL
    y = 4*eps_well*(((sig./r).^12)-((sig./r).^6));
end
```

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---

magicscatter

```
function th = magicscatter(Ec,b,V,rm,z1,z2)
%MAGICSCATTER   Outputs float value for the scattering angle from the Magic Formula.
%   Y=MAGICSCATTER(EC,B,V,RMIN,Z1,Z2) generates a float value for the
%   scattering angle using the Magic Formula.
%
%   -- EC must be the the energy in eV.
%   -- B must be the impact parameter in Angstrom.
%   -- V must be the potential function handle.
%   -- RMIN is the distance of closest approach in Angstrom.
%   -- Z1 is the atomic number of species 1.
%   -- Z2 is the atomic number of species 2.
%
%   See also RUN_SCATTERINGINTEGRALS
    m1 = 1.008; %this needs to be updated for each run!!
    m2 = 1.008; %this needs to be updated for each run!!
    a = (0.46850)/(z1^(0.23) + z2^(0.23));
    epschar = (a*Ec)/(z1*z2*14.4);
    Vprmin = zblderivative(z1,z2,rm);
    thArg = (Bvar(b,a) + Rcvar(rhovar(Ec,V(rm),Vprmin),a) +  ...
        Deltavar(epschar,Bvar(b,a),R0var(rm,a)))/(R0var(rm,a) + Rcvar(rhovar(Ec,V(rm),Vprmin),a));
    th = 2*acos(thArg);
    disp(th)
end

function y = Bvar(b,a)
    y = b/a;
end

function y = Rcvar(rhovar,a)
    y = rhovar/a;
end

function y = rhovar(E,Vrmin,Vprmin)
    y = -2*(E-Vrmin)/Vprmin;
end

function y = R0var(rmin,a)
    y = rmin/a;
end

function y = Deltavar(epschar,Bvar,R)
    C1 = 0.9923;
    C2 = 0.01162;
    C3 = 0.007122;
    C4 = 9.307;
    C5 = 14.81;
    alpha = 1 + C1/sqrt(epschar);
    beta = (C2 + sqrt(epschar))/(C3 + sqrt(epschar));
    A =2*alpha*epschar*(Bvar^beta);
```

```
    gammavar = (C4 + epschar)/(C5 + epschar);
    G = gammavar/(sqrt(1+A^2)-A);
    y = A*(R-Bvar)/(1+G);
end
```

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---

morse

```
function y = morse(rm,eps_well,k,r)
%MORSE    Outputs MORSE potential data.
%   Y=MORSE(RM,EPS_WELL,K,R) generates a float array containing
%   a potential energy value for each r value using the Morse potential.
%   Units of potential energy are eV.
%
%   -- RM must be the float distance at which the potential is at a minimum.
%   -- EPS_WELL must be the float Morse well depth.
%   -- K must be the force constant at the well minimum in units of eV/Angstrom^2.
%   -- R must be the numerical array containing r values in units of
%   Angstrom.
%
%   See also RUN_CALCPOTENTIAL
    a  = sqrt(k/(2*eps_well));
    y = eps_well*(exp(-2*a.*(r-rm))-2*exp(-a.*(r-rm)));
end
```

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---

numdiffusioncoef

```
function y = numdiffusioncoef(Tvals,m1,m2,csdatafile)
%NUMDIFFUSIONCOEF   Outputs float array with diffusion coefficient values.
%   Y=NUMDIFFUSIONCOEF(TVALS,M1,M2,P,CSDATAFILE) generates a float array
%   containing self-diffusion coefficient value for each value of Tvals by]
%   using trapezoidal integration.
%
%   -- TVALS must be an array of temperatures in Kelvin.
%   -- M1 must be mass in amu.
%   -- M2 must be mass in amu.
%   -- CSDATAFILE must be location of diffusion cross section data file.
%
%   See also NUMDIFFUSIONCS RUN_TRANSPORTCS
kb = 8.617333262E-5; %eV/K
mred = m1*m2/(m1+m2);
csdata = readmatrix(csdatafile);
Evals = csdata(:,1); %eV
csvals = csdata(:,2); %A^2
amu_to_kg = 1/(6.022e26);
ev_to_j = 1.60218e-19;
a_to_m = 1e-10;
atomic_to_si = (amu_to_kg^(-1/2))*(ev_to_j^(3/2))*(a_to_m^(-2));

y = atomic_to_si*(3/8)*((2*pi/mred)^(0.5))*((kb*Tvals).^(3/2)).*(1./(reddifquad(Tvals,Evals,csvals))); %PD in units of Pa * m^2
end
```

```
function y = reddifquad(Tvals,Evals,csvals)
kb = 8.617333262E-5; %eV/K
y = zeros(size(Tvals));
ct = 1;
for T = Tvals
    reddifintegrand = ((kb*T).^(-3)).*exp(-Evals/(kb*T)).*(Evals.^2).*csvals;
    y(ct) = trapz(Evals,reddifintegrand);
    fprintf('T = %f, omega = %f',T,y(ct)*0.5)
    ct = ct + 1;
end
end
```

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---

numdiffusioncs

```
function y = numdiffusioncs(bvals,th)
%NUMDIFFUSIONCS    Outputs diffusion cross-section value.
%   Y=NUMDIFFUSIONCS(SCATTERDATAFILE) generates diffusion cross-section
%   value by integrating scattering angle vs impact param data for a
%   specific energy using TRAPZ.
%
%   -- SCATTERDATAFILE must be the filepath to the scattering angle vs
%   impact para data.
%
%   See also RUN_TRANSPORTCS
difcsintegrand = 2*pi*(1-cos(th)).*bvals;
y = trapz(bvals,difcsintegrand);
end
```

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---

numstoppingcs

```
function y = numstoppingcs(E,m1,m2,diffusioncs)
%NUMSTOPPINGCS    Outputs stopping cross-section value.
%   Y=NUMSTOPPINGCS(SCATTERDATAFILE) generates a stopping cross-section
%   value using diffusion cs value, masses, and energy.
%
%   -- E must be energy in eV.
%   -- M1 must be the mass of species 1 in amu.
%   -- M2 must be the mass of species 2 in amu.
%   -- DIFFUSIONCS must be diffusion CS value for energy E.
%
%   See also RUN_TRANSPORTCS
yCM = 2*(m1*m2/(m1+m2)^2)*E*diffusioncs;
CMtoLab = (m1+m2)/m2;
y = yCM*CMtoLab;
end
```

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numtotalcs

```
function y = numtotalcs(th_max,bvals,th)
%NUMTOTALCS    Outputs total cross-section value.
%   Y=NUMTOTALCS(SCATTERDATAFILE) generates a total cross-section value
%   for a specific energy by finding the intersection of TH_MAX and the
%   scattering angle vs impact parameter curve.
%
%   -- TH_MAX must be the angle in radians used to determine total CS.
%   -- SCATTERDATAFILE must be the filepath to the scattering angle vs
%   impact para data.
%
%   See also RUN_TRANSPORTCS

bfine = min(bvals):0.00001:max(bvals);
th_p = th - th_max;
vqth = interp1(bvals,th_p,bfine);
bmax = max(data_zeros(bfine,vqth));
y = pi*bmax^2;
end

function x0 = data_zeros(x, y)
    % Identify indices where there is a sign change between consecutive elements
    zero_crossings = find((y(1:end-1) .* y(2:end)) <= 0);

    % Preallocate for the zero-crossing points
    x0 = NaN(length(zero_crossings), 1);

    % Loop through each detected zero-crossing for interpolation
    for k = 1:length(zero_crossings)
        % Indices for interpolation points
        idx1 = zero_crossings(k);
        idx2 = idx1 + 1;

        % Linear interpolation between the points around zero-crossing
        b = [1, x(idx1); 1, x(idx2)] \ [y(idx1); y(idx2)];
        x0(k) = -b(1) / b(2); % Solving for x at y = 0
    end
    x0 = x0(~isnan(x0));
end
```

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numtotalcscheb

```
function y = numtotalcscheb(th_max,bvals,th)
%NUMTOTALCSCHEB    Outputs total cross-section value.
%   Y=NUMTOTALCSCHEB(SCATTERDATAFILE) generates a total cross-section value
%   for a specific energy by finding the intersection of TH_MAX and the
%   scattering angle vs impact parameter curve using Chebfun rootfinding.
%
%   -- TH_MAX must be the angle in radians used to determine total CS.
%   -- SCATTERDATAFILE must be the filepath to the scattering angle vs
%   impact para data.
%
%   See also RUN_TRANSPORTCS
th_p = th - th_max;
```

```
p = spline(bvals,th_p);
poly = @(r) ppval(p,r);
chebtotalcs = chebfun(poly,[min(bvals),max(bvals)]);
bmax = max(roots(chebtotalcs));
y = pi*bmax^2;
end
```

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---

numvisccoef

```
function y = numvisccoef(Tvals,m1,m2,csdatafile)
%NUMVISCCOEF   Outputs float array with viscosity coefficient values.
%   Y=NUMVISCCOEF(TVALS,M1,M2,CSDATAFILE) generates a float array
%   containing viscosity coefficient value for each value of Tvals by using
%   trapezoidal integration.
%
%   -- TVALS must be an array of temperatures in Kelvin.
%   -- M1 must be mass in amu.
%   -- M2 must be mass in amu.
%   -- CSDATAFILE must be location of viscosity cross section data file.
%
%   See also NUMDIFFUSIONCOEF RUN_TRANSPORTCS
kb = 8.617333262E-5; %eV/K
mred = m1*m2/(m1+m2);
csdata = readmatrix(csdatafile);
Evals = csdata(:,1); %eV
csvals = csdata(:,2); %A^2
% note that the 0.001629989 below is a unit conversion factor that converts
% [amu^0.5 * Angstrom^-2 * eV^0.5] --> [kg^0.5 * m^-2 * Joules^0.5]
y = (1E6)*0.001629989*(5/4)*((2*pi*mred)^(0.5))*((kb*Tvals).^(1/2)).*(1./(redviscquad(Tvals,Evals,csvals))); %microPa s
end

function y = redviscquad(Tvals,Evals,csvals)
kb = 8.617333262E-5; %eV/K
y = zeros(size(Tvals));
ct = 1;
for T = Tvals
    redviscintegrand = ((kb*T).^(-4)).*exp(-Evals/(kb*T)).*(Evals.^3).*csvals;
    y(ct) = trapz(Evals,redviscintegrand);
    ct = ct + 1;
end
end
```

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---

numvisccs

```
function y = numvisccs(bvals,th)
%NUMVISCCS    Outputs viscosity cross-section value.
%   Y=NUMVISCCS(SCATTERDATAFILE) generates a viscosity cross-section
%   value by integrating scattering angle vs impact param data for a
%   specific energy using TRAPZ.
%
```

```
%   -- SCATTERDATAFILE must be the filepath to the scattering angle vs
%   impact para data.
%
%   See also RUN_TRANSPORTCS
difcsintegrand = 2*pi*(1-cos(th).^2).*bvals;
y = trapz(bvals,difcsintegrand);
end
```

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---

powerlaw

```
function y = powerlaw(a,k,r)
%POWERLAW    Outputs power law potential data.
%   Y=POWERLAW(A,K,R) generates a float array containing a potential
%   energy value for each r value using the basic power law potential.
%   Units of potential energy are eV.
%
%   -- A is the first power law coefficient.
%   -- K is the exponent power law coefficient.
%   -- R must be the numerical array containing r values in units of
%   Angstrom.
%
%   See also RUN_CALCPOTENTIAL
    y = a*r.^(-k);
end
```

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---

run_calcpotential

```
function y = run_calcpotential(filepath,datafilepath)
%RUN_CALCPOTENTIAL    Reads input file and generates potential data.
%   RUN_CALCPOTENTIAL(FILEPATH,DATAFILEPATH) reads the user-specified input
%   file, generates potential data using the appropriate potential
%   function, and saves the data to a user-specified folder.
%
%   -- FILEPATH must specify the path to where input file is.
%   -- DATAFILEPATH must specify where to save the potential data.
%
%   See also COULOMB LJ_126 LJ_124 ZBL POWERLAW MORSE
    run(filepath);
    r = minR:Rstep:maxR;
    if strcmp(Potential_Type,"Coulomb")
        data = coulomb(Z1,Z2,r);
        datapath  = fullfile(datafilepath,'/coulombdata.csv');
        A = [r' data'];
        writematrix(A,datapath);
        y = datapath;
    elseif strcmp(Potential_Type,"12-6 Lennard-Jones")
        data = lj_126(eps_well,sig,r);
        datapath  = fullfile(datafilepath,'/126ljdata.csv');
        A = [r' data'];
        writematrix(A,datapath);
```

```
        y = datapath;
    elseif strcmp(Potential_Type,"12-4 Lennard-Jones")
        data = lj_124(eps_well,sig,r);
        datapath  = fullfile(datafilepath,'/124ljdata.csv');
        A = [r' data'];
        writematrix(A,datapath);
        y = datapath;
    elseif strcmp(Potential_Type,"ZBL")
        data = zbl(Z1,Z2,r);
        datapath  = fullfile(datafilepath,'/zbldata.csv');
        A = [r' data'];
        writematrix(A,datapath);
        y = datapath;
    elseif strcmp(Potential_Type,"Morse")
        data = morse(rm,eps_well,k,r);
        datapath  = fullfile(datafilepath,'/morsedata.csv');
        A = [r' data'];
        writematrix(A,datapath);
        y = datapath;
    elseif strcmp(Potential_Type,"Power Law")
        data = powerlaw(a,k,r);
        datapath = fullfile(datafilepath,'/powerlawdata.csv');
        A = [r' data'];
        writematrix(A,datapath);
        y = datapath;
    end
end
```

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---

run_dsmccoef

```
function y = run_dsmccoef(inputfile,datapath)
%RUN_DSMCCOEF    Reads dsmc coef input file and calculates dsmc params.
%   RUN_DSMCCOEF(INPUTFILE,DATAPATH) reads the user-specified parameters
%   from the input file and calculates DSMC params for the VSS and VHS
%   models.
%
%   -- INPUTFILE must specify the path to where input file is.
%   -- DATAFILEPATH must specify where to save the param table.
%
%   See also VHSCOEF VHSVISCOSITY VSSCOEF VSSDIFFUSION
y = datapath;
run(inputfile);
mr = m1*m2/(m1+m2);
mrkg = mr/(6.022E26);
kb = 1.380649E-23; %J/K
cd(sprintf('%s',y))
mkdir dsmcfitdata
visccoefdata = readmatrix(viscdatafile);
visccoef = visccoefdata(:,2);
Tvals = visccoefdata(:,1);
Tfine = min(Tvals):0.01:max(Tvals);
vqvisc = interp1(Tvals,visccoef,Tfine);
delta = (max(Tvals) - min(Tvals))/N;
offset = min(Tvals);
dsmcdatapath = fullfile(datapath,'/dsmccoeftable.csv');
A = [];
```

```
C = [Tfine' vqvisc'];
interpviscdata = fullfile(datapath,'/dsmcfitdata/dsmcfitviscdata.csv');
writematrix(C,interpviscdata);
for i = 1:N
    minT = offset;
    maxT = minT + delta;
    excludeT = ((Tfine < minT) | (Tfine > maxT));
    fitT = Tfine;
    fitT(excludeT) = [];
    T_sample = 0.5*(minT + maxT);
    vhscoefs = my_VHScoef(fitT,T_sample,excludeT,vqvisc,tol);
    mu_sample = vhscoefs(1);
    omega = vhscoefs(2);
    dcollision = (1E10)*sqrt(15*sqrt(mrkg*kb*T_sample/pi)/...
        (2*(5-2*omega)*(7-2*omega)*(mu_sample/(1E6)))); %Angstrom
    viscfit = my_VHSviscosity(fitT,omega,T_sample,mu_sample);
    viscfitdatapath = fullfile(datapath,sprintf('/dsmcfitdata/viscfitdata_n=%i.csv',i));
    B1 = [fitT' viscfit'];
    writematrix(B1,viscfitdatapath);
    A = [A; minT maxT mu_sample T_sample omega dcollision];
    offset  = offset + delta;
end
A = array2table(A,'VariableNames',{'Tmin','Tmax','mu_ref','T_ref','omega','collision_diam'});
disp(A)
writetable(A,dsmcdatapath);
end
```

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---

run_fitpotential

```
function y = run_fitpotential(filepath,datapath)
%RUN_FITPOTENTIAL    Reads fitting input file and generates cfit object.
%   RUN_FITPOTENTIAL(FILEPATH,DATAFILEPATH) reads the user-specified
%   fitting parameters from the fitting input file, creates a fittype based
%   off those parameters using the appropriate character function or
%   string, and then creates a fit object using the FIT function.
%
%   -- FILEPATH must specify the path to where input file is.
%   -- DATAFILEPATH must specify where the potential data is saved.
%
%   See also COULOMBCHAR ZBLCHAR
    run(filepath);
    if strcmp(Potential_Type,"Coulomb")
        ft = fittype(coulombchar(Z1),dependent="y",independent="x",...
        coefficients="z2");
        t = readmatrix(datapath);
        excludex = ((t(:,1) < minR) | (t(:,1) > maxR));
        xvals = t(:,1);
        yvals = t(:,2);
        xvals(excludex) = [];
        yvals(excludex) = [];
        y = fit(xvals,yvals,ft,'Exclude',(xvals<minR)&(xvals>maxR),...
            'TolFun',tol,'Lower',minZ2,'Upper',maxZ2);
    elseif strcmp(Potential_Type,"ZBL")
        ft = fittype(zblchar(Z1),dependent="y",independent="x",...
        coefficients="z2");
        t = readmatrix(datapath);
```

```
        excludex = ((t(:,1) < minR) | (t(:,1) > maxR));
        xvals = t(:,1);
        yvals = t(:,2);
        xvals(excludex) = [];
        yvals(excludex) = [];
        y = fit(xvals,yvals,ft,'Exclude',(xvals<minR)&(xvals>maxR),...
            'TolFun',tol,'Lower',minZ2,'Upper',maxZ2);
    elseif strcmp(Potential_Type,"12-6 Lennard-Jones")
        t = readmatrix(datapath);
        excludex = ((t(:,1) < minR) | (t(:,1) > maxR));
        xvals = t(:,1);
        yvals = t(:,2);
        xvals(excludex) = [];
        yvals(excludex) = [];
        ft = fittype("4*eps_well*(((sigma./x).^12)-((sigma./x).^6))",dependent="y",...
                    independent="x",coefficients=["eps_well" "sigma"]);
        y = fit(xvals,yvals,ft,...
                    'TolFun',tol,'Lower',[min_eps min_sigma],...
                    'Upper',[max_eps max_sigma],'StartPoint',[eps_start sigma_start]);
    elseif strcmp(Potential_Type,"12-4 Lennard-Jones")
        t = readmatrix(datapath);
        excludex = ((t(:,1) < minR) | (t(:,1) > maxR));
        xvals = t(:,1);
        yvals = t(:,2);
        xvals(excludex) = [];
        yvals(excludex) = [];
        ft = fittype("0.5*(3^1.5)*eps_well*(((sigma./x).^12)-((sigma./x).^4))",dependent="y",...
                    independent="x",coefficients=["eps_well" "sigma"]);
        y = fit(xvals,yvals,ft,...
                    'TolFun',tol,'Lower',[min_eps min_sigma],...
                    'Upper',[max_eps max_sigma],'StartPoint',[eps_start sigma_start]);
    elseif strcmp(Potential_Type,"Morse")
        t = readmatrix(datapath);
        excludex = ((t(:,1) < minR) | (t(:,1) > maxR));
        xvals = t(:,1);
        yvals = t(:,2);
        xvals(excludex) = [];
        yvals(excludex) = [];
        ft = fittype("eps_well*(exp(-2*sqrt(k/(2*eps_well)).*(x-rm))-2*exp(-sqrt(k/(2*eps_well)).*(x-rm)))", ...
            dependent="y",independent="x",coefficients=["rm" "eps_well" "k"]);
        y = fit(xvals,yvals,ft,...
                    'TolFun',tol,'Lower',[min_rm min_eps min_k],...
                    'Upper',[max_rm max_eps max_k],'StartPoint',[rm_start eps_start k_start]);
    elseif strcmp(Potential_Type,"Power Law")
        t = readmatrix(datapath);
        excludex = ((t(:,1) < minR) | (t(:,1) > maxR));
        xvals = t(:,1);
        yvals = t(:,2);
        xvals(excludex) = [];
        yvals(excludex) = [];
        ft = fittype("a*x.^(-k)",dependent="y",...
                    independent="x",coefficients=["a" "k"]);
        y = fit(xvals,yvals,ft,...
                    'TolFun',tol,'Lower',[min_a min_k],...
                    'Upper',[max_a max_k],'StartPoint',[a_start k_start]);
    end
end
```

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run_scatteringintegrals

```
function y = run_scatteringintegrals(filepath,datafilepath,progressBar)
%RUN_SCATTERINGINTEGRALS    Reads scattering input file and calculates scattering integrals.
%   RUN_SCATTERINGINTEGRALS(FILEPATH,DATAFILEPATH) reads the user-specified
%   scattering parameters from the scattering input file and calculates the
%   differential scattering cross section, impact parameter, and distance
%   of closest approach (for the Coulomb case), or calculates the
%   scattering angle and distance of closest approach (general) case.
%
%   -- FILEPATH must specify the path to where input file is.
%   -- DATAFILEPATH must specify where to save the scattering integral data.
%
%   See also IMPACT DIFSCATTER DISTCLOSE DOCAROOT GMQUADSCATTERINGANGLE
    y = datafilepath;
    run(filepath);
    if logspace_on == 1
        minElog = log10(minE);
        maxElog = log10(maxE);
        Evals = logspace(minElog,maxElog,logstep);
    elseif logspace_on == 0
        Evals = minE:Estep:maxE;
    end
    cd(sprintf('%s',y))

    if strcmp(inttype,'Exact Coulomb')
        theta = theta_min:theta_step:theta_max;
        numESteps = numel(Evals);
        numthSteps = numel(theta);
        A = zeros(numthSteps,numESteps);
        B = zeros(numthSteps,numESteps);
        C = zeros(numthSteps,2*numESteps);
        colNames = strings(1,1+numESteps);
        A(:,1) = theta';
        B(:,1) = theta';
        colNames(1,1) = 'theta';
        colNamesC = strings(1,2*numESteps);
        for i = 1:numESteps
            E = Evals(i);
            if nargin > 2 && isvalid(progressBar)
                progressBar.Value = i / numESteps;
                progressBar.Message = sprintf('Running %f eV...', E);
            end
            mydifscatter = difscatter(Z1, Z2, theta, E);
            impactparam = impact(Z2, Z2, theta, E);
            doca = distclose(Z1, Z2, impactparam, E);
            colNames(i+1) = sprintf('E=%f',E);
            colNamesC(1,2*i-1) = sprintf('bval E=%f',E);
            colNamesC(1,2*i) = sprintf('doca E=%f',E);
            A(:,i+1) = mydifscatter';
            B(:,i+1) = impactparam';
            C(:,2*i-1) = impactparam';
            C(:,2*i) = doca';
        end
        ATable = array2table(A,'VariableNames',colNames);
        BTable = array2table(B,'VariableNames',colNames);
        CTable = array2table(C,'VariableNames',colNamesC);
        difscatterdatapath = fullfile(datafilepath,'/difscatterdata.csv');
        impactparamdatapath = fullfile(datafilepath,'/impactparamdata.csv');
        docadatapath = fullfile(datafilepath,'/docadata.csv');
        writetable(ATable, difscatterdatapath);
```

```
    writetable(BTable, impactparamdatapath);
    writetable(CTable, docadatapath);

elseif strcmp(inttype, 'Numerical')
    run(fitfile);
    if strcmp(Potential_Type, 'Coulomb')
        potential = @(r) coulomb(Z1, z2_param, r);
    elseif strcmp(Potential_Type, '12-6 Lennard-Jones')
        potential = @(r) lj_126(eps_param, sigma_param, r);
    elseif strcmp(Potential_Type, '12-4 Lennard-Jones')
        potential = @(r) lj_124(eps_param, sigma_param, r);
    elseif strcmp(Potential_Type, 'ZBL')
        potential = @(r) zbl(Z1, z2_param, r);
    elseif strcmp(Potential_Type, 'Morse')
        potential = @(r) morse(rm_param,eps_param,k_param,r);
    elseif strcmp(Potential_Type, 'Power Law')
        potential = @(r) powerlaw(a_param, k_param, r);
    end
    if blogspace_on == 1
        minblog = log10(bmin);
        maxblog = log10(bmax);
        bvals = logspace(minblog,maxblog,blogstep);
    elseif blogspace_on == 0
        bvals = bmin:bstep:bmax;
    end

    numESteps = numel(Evals);
    numBSteps = numel(bvals);
    A = zeros(numBSteps,numESteps);
    B = zeros(numBSteps,numESteps);
    colNames = strings(1,1+numESteps);
    A(:,1) = bvals';
    B(:,1) = bvals';
    colNames(1,1) = 'bvals';

    for i = 1:numESteps
        E = Evals(i);
        if nargin > 2 && isvalid(progressBar)
            progressBar.Value = i / numESteps;
            progressBar.Message = sprintf('Running %f eV...', E);
        end
        docas = zeros(1, length(bvals));
        th = zeros(1, length(bvals));
        thmagic = zeros(1,length(bvals));
        for j = 1:length(bvals)
            docas(j) = DOCAroot(E, bvals(j), potential, minroot, maxroot,chebfunpath);
            th(j) = GMquadScatteringAngle(potential, E, bvals(j), docas(j), 20);
            if strcmp(Potential_Type, 'ZBL')
                thmagic(j) = magicscatter(E,bvals(j),potential,docas(j),Z1,z2_param);
            end
        end
        colNames(i+1) = sprintf('E=%f',E);
        A(:,i+1) = th';
        B(:,i+1) = docas';
        C = [bvals' thmagic'];
        %magicscatterpath = fullfile(datafilepath,sprintf('/magicscatterdata/scatterangledata_%f.csv',E));
        %writematrix(C, magicscatterpath)
    end
    ATable = array2table(A,'VariableNames',colNames);
    BTable = array2table(B,'VariableNames',colNames);
    scatterangdatapath = fullfile(datafilepath,'/scatterangledata.csv');
    docadatapath = fullfile(datafilepath,'/docadata.csv');
```

```
        writetable(ATable, scatterangdatapath);
        writetable(BTable, docadatapath);
        %writematrix(C, magicscatterpath)
    end
end
```

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---

run_transportCS

```
function run_transportCS(filepath,datafilepath)
%RUN_TRANSPORTCS    Reads cross-section input file and calculates transport cross-sections.
%   RUN_TRANSPORTCS(FILEPATH,DATAFILEPATH) reads the user-specified
%   cross-section (CS) parameters from the cross-section input file and
%   calculates the diffusion CS and viscosity CS (for the exact LJ case in
%   "Khrapak, S.A. Accurate transport cross sections for the Lennard-Jones
%   potential. Eur. Phys. J. D 68, 276 (2014)") or the diffusion CS,
%   viscosity CS, stopping CS, and total CS (for the general case).
%
%   -- FILEPATH must specify the path to where input file is.
%   -- DATAFILEPATH must specify where to save the CS data.
%
%   See also DIFFUSIONCS VISCOSITYCS NUMDIFFUSIONCS NUMVISCCS
%   NUMTOTALCS NUMSTOPPINGCS
    run(filepath);
    if logspace_on == 1
        minElog = log10(minE);
        maxElog = log10(maxE);
        Evals = logspace(minElog,maxElog,logstep);
    elseif logspace_on == 0
        Evals = minE:Estep:maxE;
    end
    if strcmp(inttype,'Exact LJ')
        beta = welldepth./(2*Evals);
        difcs = diffusioncs(beta);
        visccs = viscositycs(beta);
        A = [Evals' difcs'];
        B = [Evals' visccs'];

    elseif strcmp(inttype,'Numerical')
        difcs = zeros(1,length(Evals));
        visccs = zeros(1,length(Evals));
        stoppingcs = zeros(1,length(Evals));
        totalcs = zeros(1,length(Evals));
        for j = 1:length(Evals)
            disp(Evals(j))
            file = datafile;
            scatterdata = readmatrix(file);
            th = scatterdata(:,j+1);
            bvals = scatterdata(:,1);
            if strcmp(thetacutoff,'Quantum')
                docadata = readmatrix(docafile);
                doca = docadata(:,j+1)*(1e-10); %m
                hbar = 1.054571817E-34; %J*s
                m_redamu  = m1*m2/(m1+m2);
                m_red = m_redamu/(6.022E26); %kg
                E = Evals(j)*(1.60218E-19); %J
                v_cm = sqrt(2*E/m_red);
```

```
                lam_bar = hbar/(m_red*v_cm);
                th_c = lam_bar./doca;
            elseif strcmp(thetacutoff,'Manual')
                th_c = th_max;
            end
            difcs(j) = numdiffusioncs(bvals,th);
            visccs(j) = numvisccs(bvals,th);
            stoppingcs(j) = numstoppingcs(Evals(j),m1,m2,diffusioncs(j));
            totalcs(j) = numtotalcs(th_c,bvals,th);
        end
        CMtoLab = (m1+m2)/m2;
        A = [Evals' difcs'];
        B = [Evals' visccs'];
        C = [(CMtoLab*Evals)' stoppingcs'];
        D = [Evals' totalcs'];
        stoppingcsdatapath = fullfile(datafilepath,'/stoppingcsdata.csv');
        totalcsdatapath = fullfile(datafilepath,'/totalcsdata.csv');
        writematrix(C,stoppingcsdatapath);
        writematrix(D,totalcsdatapath);
    end
    diffusioncsdatapath  = fullfile(datafilepath,'/diffusioncsdata.csv');
    viscositycsdatapath = fullfile(datafilepath,'/viscositycsdata.csv');
    writematrix(A, diffusioncsdatapath);
    writematrix(B,viscositycsdatapath);

end
```

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---

run_transportcoefs

```
function y = run_transportcoefs(filepath,datafilepath)
%RUN_TRANSPORTCOEFS    Reads transport input file and calculates transport coefs.
%   RUN_TRANSPORTCOEFS(FILEPATH,DATAFILEPATH) reads the user-specified
%   transport parameters from the transport input file and calculates the
%   self-diffusion or viscosity coefficient.
%
%   -- FILEPATH must specify the path to where input file is.
%   -- DATAFILEPATH must specify where to save the coef data.
%
%   See also DIFFUSIONCOEF VISCCOEF NUMDIFFUSIONCOEF NUMVISCCOEF
    %disp(filepath)
    run(filepath);
    Tvals = minT:Tstep:maxT;
    if strcmp(inttype,'Exact LJ') | strcmp(inttype,'Trapezoidal LJ')
            difcoef = diffusion_coef(welldepth,Tvals,m1,m2,d,inttype,diffusiondatafile);
            diffusioncoefdatapath  = fullfile(datafilepath,'/diffusioncoefdata.csv');
            A = [Tvals' difcoef'];
            writematrix(A, diffusioncoefdatapath);
            viscositycoef = visc_coef(welldepth,Tvals,m1,m2,d,inttype,viscositydatafile);
            visccoefdatapath  = fullfile(datafilepath,'/viscositycoefdata.csv');
            B = [Tvals' viscositycoef'];
            writematrix(B, visccoefdatapath);
            y = datafilepath;
    elseif strcmp(inttype,'Numerical')
            diffusioncoef = numdiffusioncoef(Tvals,m1,m2,diffusiondatafile);
            diffusioncoefdatapath  = fullfile(datafilepath,'/diffusioncoefdata.csv');
            A = [Tvals' diffusioncoef'];
```

```
            writematrix(A, diffusioncoefdatapath);
            visccoef = numvisccoef(Tvals,m1,m2,viscositydatafile);
            visccoefdatapath  = fullfile(datafilepath,'/viscositycoefdata.csv');
            B = [Tvals' visccoef'];
            writematrix(B, visccoefdatapath);
            coefdatapath = datafilepath;
            y = coefdatapath;
    end
end
```

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---

run_vhscoef

```
function y = run_vhscoef(inputfile,datapath)
%RUN_VHSCOEF    Reads VHS coef input file and calculates VHS params.
%   RUN_DSMCCOEF(INPUTFILE,DATAPATH) reads the user-specified parameters
%   from the input file and calculates DSMC params for the VHS
%   model.
%
%   -- INPUTFILE must specify the path to where input file is.
%   -- DATAFILEPATH must specify where to save the param table.
%
%   See also VHSCOEF VHSVISCOSITY
y = datapath;
run(inputfile);
%mr = m1*m2/(m1+m2);
mr = m1;
mrkg = mr/(6.022E26);
kb = 1.380649E-23; %J/K
cd(sprintf('%s',y))
mkdir vhsfitdata
visccoefdata = readmatrix(viscdatafile);
visccoef = visccoefdata(:,2);
Tvals = visccoefdata(:,1);
Tfine = min(Tvals):0.01:max(Tvals);
vqvisc = interp1(Tvals,visccoef,Tfine);
delta = (max(Tvals) - min(Tvals))/N;
offset = min(Tvals);
vhsdatapath = fullfile(datapath,'/vhscoeftable.csv');
A = [];
C = [Tfine' vqvisc'];
interpviscdata = fullfile(datapath,'/vhsfitdata/vhsfitviscdata.csv');
writematrix(C,interpviscdata);
for i = 1:N
    minT = offset;
    maxT = minT + delta;
    excludeT = ((Tfine < minT) | (Tfine > maxT));
    fitT = Tfine;
    fitT(excludeT) = [];
    T_sample = 0.5*(minT + maxT);
    mu_sample = interp1(Tfine, vqvisc, T_sample);
    vhscoefs = VHScoef(fitT,T_sample,mu_sample,excludeT,vqvisc,tol);
    omega = vhscoefs(2);
    dcollision = (1E10)*sqrt(15*sqrt(mrkg*kb*T_sample/pi)/...
        (2*(5-2*omega)*(7-2*omega)*(mu_sample/(1E6)))); %Angstrom
    viscfit = VHSviscosity(fitT,omega,T_sample,mu_sample);
    viscfitdatapath = fullfile(datapath,sprintf('/vhsfitdata/viscfitdata_n=%i.csv',i));
```

```
    B1 = [fitT' viscfit'];
    writematrix(B1,viscfitdatapath);
    A = [A; minT maxT mu_sample T_sample omega dcollision];
    offset  = offset + delta;
end
A = array2table(A,'VariableNames',{'Tmin','Tmax','mu_ref','T_ref','omega','collision_diam'});
disp(A)
writetable(A,vhsdatapath);
end
```

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---

run_vsscoef

```
function y = run_vsscoef(inputfile,datapath)
%RUN_VSSCOEF    Reads VSS coef input file and calculates VSS params.
%   RUN_DSMCCOEF(INPUTFILE,DATAPATH) reads the user-specified parameters
%   from the input file and calculates DSMC params for the VSS
%   model.
%
%   -- INPUTFILE must specify the path to where input file is.
%   -- DATAFILEPATH must specify where to save the param table.
%
%   See also VSSALPHA VSSDIAMETER VSSCONVERGENCE
y = datapath;
run(inputfile);
%mr = m1*m2/(m1+m2);
mr = m1;
mrkg = mr/(6.022E26);
molarkg = mr/(1E3);
difcoefdata = readmatrix(diffusiondatafile);
vhscoefdata = readmatrix(vhstablefile);
viscvals = vhscoefdata(:,3)*(1E-6);
omegavals = vhscoefdata(:,5);
alphavals = alphaguess*ones(length(omegavals),1);
Tvals = vhscoefdata(:,4);
difcoef = difcoefdata(:,2);
difcoef_T = difcoefdata(:,1);
dif_sample = interp1(difcoef_T, difcoef, Tvals);
max_iter = 100;
iter = 0;
while VSSconvergence(alphavals,omegavals,molarkg,Tvals,dif_sample,viscvals,tol) && iter < max_iter
diams = VSSdiameter(alphavals,omegavals,mrkg,Tvals,viscvals);
newalpha = VSSalpha(omegavals,mrkg,molarkg,Tvals,dif_sample,diams);
alphavals = newalpha;
iter = iter + 1;
end
if iter == max_iter
    warning('Reached maximum number of iterations without convergence.');
end
diams = VSSdiameter(alphavals,omegavals,mrkg,Tvals,viscvals);
diams_angstrom  = diams*(1E10);
A = [Tvals alphavals diams_angstrom];
vssdatapath = fullfile(datapath,'/VSScoeftable.csv');
A = array2table(A,'VariableNames',{'Reference Temp (K)', 'alpha','collision_diam'});
disp(A)
writetable(A,vssdatapath);
end
```

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visc_coef

```
function y = visc_coef(well_depth,T,m1,m2,d,inttype,data)
%VISC_COEF    Outputs viscosity coefficient.
%   Y=VISC_COEF(WELL_DEPTH,T,M1,M2,D,INTTYPE,DATA) generates a float
%   array containing a viscosity coefficient value for each temperature
%   using a Lennard_Jones potential (from "Khrapak, S.A. Accurate transport
%   cross sections for the Lennard-Jones potential. Eur. Phys. J. D 68, 276
%   (2014)"). Units of viscosity coefficient are micro-Pascal*s.
%
%   -- WELL-DEPTH must be the LJ well-depth in Kelvin.
%   -- T must be a float array containing temperature values in units of K.
%   -- M1 must be the mass of species 1 in amu.
%   -- M2 must be the mass of species 2 in amu.
%   -- D must be the sigma LJ parameter in units of Angstrom.
%   -- INTTYPE must be a character string specifying if the integral will
%   be exact or numerical.
%   -- DATA must be a character string filepath that gives the location of
%   the cross section data.
%
%   See also RUN_TRANSPORTCS
Tjoul = T.*(1.380649e-23);
mu = (m1*m2)/(m1+m2);
mukg = mu*(1.66054e-27);
dm = d*(1e-10);
Tstar = T/well_depth;
if strcmp(inttype,'Exact LJ')
y = (1e6)*(5*sqrt(2*pi)/8)*(((mukg)^(1/2))*(Tjoul).^(1/2))./(((dm)^2) ...
    *reducedviscint(Tstar));
elseif strcmp(inttype,'Trapezoidal LJ')
y = (1e6)*(5*sqrt(2*pi)/8)*(((mukg)^(1/2))*(Tjoul).^(1/2))./(((dm)^2) ...
    *reducedviscquad(Tstar,data));
else
    disp('Invalid Integration Type. Please check input file and try again.')
end
end

function y = reducedviscint(Tstar)
%REDUCEDVISCINT    Outputs the reduced viscosity integral.
%   Y=MY_REDUCEDVISCINT(TSTAR) generates a float array containing a value
%   for the exact reduced viscosity integral in Khrapak, S.A. Accurate
%   transport cross sections for the Lennard-Jones potential (2014).
%
%   -- TSTAR is  float array containing the reduced temperature values.
y = zeros(size(Tstar));
ct = 1;
for t = Tstar
redviscintegrand = @(x) 0.5*(x.^3).*exp(-x).*viscositycs(1./(2*t*x));
y(ct) = integral(redviscintegrand,0,Inf);
ct = ct + 1;
end
end

function y = reducedviscquad(Tstar,data)
%REDUCEDVISCQUAD    Outputs the reduced viscosity integral using quadrature.
%   Y=MY_REDUCEDVISCQUAD(TSTAR,DATA) generates a float array containing a value
%   for the reduced viscosity integral in Khrapak, S.A. Accurate transport
```

```
%   cross sections for the Lennard-Jones potential (2014) using trapezoidal
%   integration.
%
%   -- TSTAR is  float array containing the reduced temperature values.
%   -- DATA is a char array containing the filepath of the cross-section
%   data.
y = zeros(size(Tstar));
ct = 1;
csdata = readmatrix(data);
for t = Tstar
X = 1./(2*t*csdata(:,1));
redviscintegrand = -0.25*(X.^3).*exp(-X).*csdata(:,2)./(t*csdata(:,1).^2);
y(ct) = trapz(csdata(:,1),redviscintegrand);
ct = ct + 1;
end
end
```

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viscositycs

```
function y = viscositycs(beta)
%VISCOSITYCS    Outputs float array with viscosity cross-section values.
%   Y=VISCOSITYCS(BETA) generates a float array containing viscosity
%   cros-section value for each value of the scattering parameter beta
%   using a Lennard_Jones potential.
%
%   -- BETA must be a float array containing values for the dimensionless
%   scattering parameter.
%
%   See also DIFFUSIONCS RUN_TRANSPORTCS
fLEeta = 1;
fHEeta = 1 - 2.229.*(beta) + 35.967.*(beta.^(2)) - 86.490.*(beta.^(3)) ...
    + 60.335.*(beta.^(4));

y = zeros(size(beta));
%%Case 1: beta < 0.491
idx1 = beta < 0.491;
y(idx1) = 3.599.*(beta(idx1).^(1/6)).*fHEeta(idx1);

%%Case 2: beta > 0.491
idx2 = beta > 0.491;
y(idx2) = 7.480.*(beta(idx2).^(1/3))*fLEeta;
end
```

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zbl

```
function y = zbl(z1,z2,r)
%ZBL    Outputs ZBL potential data.
%   Y=ZBL(Z1,Z2,R) generates a float array containing
%   a potential energy value for each r value using the ZBL potential.
%   Units of potential energy are eV.
```

```
%
%   -- Z1 must be the integer atomic number of species 1.
%   -- Z2 must be the integer atomic number of species 2.
%   -- R must be the numerical array containing r values in units of
%   Angstrom.
%
%   See also RUN_CALCPOTENTIAL
    eps_naught = 0.005526349406; %e^2 * eV^-1 * Angstrom^-1
    Ke = 4*pi*eps_naught;
    a = (0.46850)/(z1^(0.23) + z2^(0.23));
    y = phi(r/a).*z1*z2./(Ke.*r);
end

function y = phi(x)
    y = 0.18175*exp(-3.19980*x) + 0.50986*exp(-0.94229*x) + ...
        0.28022*exp(-0.40290*x) + 0.02817*exp(-0.20162*x);
end
```

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---

zblchar

```
function y = zblchar(z1)
%ZBLCHAR    Outputs character array with fitting model.
%   Y=ZBLCHAR(Z1) generates a char array containing the ZBL potential
%   equation with the user-specified Z1.
%
%   -- Z1 must be the integer atomic number of species 1.
%
%   See also RUN_FITPOTENTIAL
    eps_naught = 0.005526349406; %e^2 * eV^-1 * Angstrom^-1
    Ke = 1/(4*pi*eps_naught);
    a = sprintf('(0.46850)/((%i)^(0.23) + z2^(0.23))',z1);
    phi1 = sprintf('0.18175*exp(-3.19980*x/(%s)) + 0.50986*exp(-0.94229*x/(%s))',a,a);
    phi2 = sprintf('0.28022*exp(-0.40290*x/(%s)) + 0.02817*exp(-0.20162*x/(%s))',a,a);
    phi = [phi1 '+' phi2];
    y = sprintf("(%d)*(%s)*%i*z2./x",Ke,phi,z1);
end
```

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---

zblderivative

```
function y = zblderivative(z1,z2,r)
%ZBLDERIVATIVE    Outputs the derivative of a ZBL potential.
%   Y=ZBLDERIVATIVE(Z1,Z2,R) generates a float array containing
%   the derivative of the potential energy for each r value using the ZBL potential.
%   Units of potential energy are eV.
%
%   -- Z1 must be the integer atomic number of species 1.
%   -- Z2 must be the integer atomic number of species 2.
%   -- R must be the numerical array containing r values in units of
%   Angstrom.
%
```

```
%   See also RUN_CALCPOTENTIAL
    eps_naught = 0.005526349406; %e^2 * eV^-1 * Angstrom^-1
    k = 1/(4*pi*eps_naught);
    a = (0.46850)/(z1^(0.23) + z2^(0.23));
    y = (-k*z1*z2./(r.^2))*(0.18175*exp(-3.19980*r/a) + 0.50986*exp(-0.94229*r/a) + ...
        0.28022*exp(-0.40290*r/a) + 0.02817*exp(-0.20162*r/a)) + ...
        (k*z1*z2./(r*a))*((0.18175*-3.19980)*exp(-3.19980*r/a) + (0.50986*-0.94229)*exp(-0.94229*r/a) + ...
        (0.28022*-0.40290)*exp(-0.40290*r/a) + (0.02817*-0.20162)*exp(-0.20162*r/a));
end
```

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