Tutorial on First Principles Equation of state (FPEOS) database

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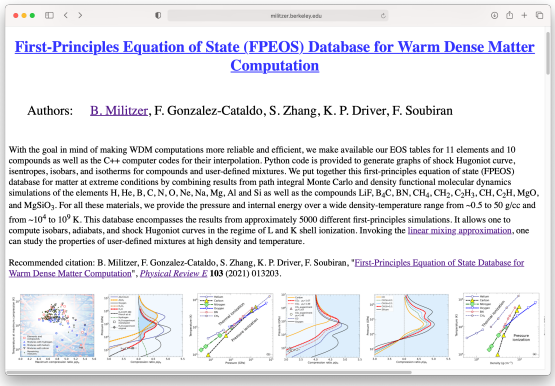
(1) Go to **http://militzer.berkeley.edu/FPEOS**, download the latest version, **fpeos_05-21-24.tar.gz**, and install it on your computer following the installation instruction on the website.



First-Principles Equation of State (FPEOS) Database for Warm Dense Matter Computation

Authors: B. Militzer, F. Gonzalez-Cataldo, S. Zhang, K. P. Driver, F. Soubiran

With the goal in mind of making WDM computations more reliable and efficient, we make available our EOS tables for 11 elements and 10 compounds as well as the C++ computer codes for their interpolation. Python code is provided to generate graphs of shock Hugoniot curve, isentropes, isobars, and isotherms for compounds and user-defined mixtures. We put together this first-principles equation of state (FPEOS) database for matter at extreme conditions by combining results from path integral Monte Carlo and density functional molecular dynamics simulations of the elements H, He, B, C, N, O, Ne, Na, Mg, Al and Si as well as the compounds LiF, B_4C, BN, CH_4, CH_2, C_2H_3, CH, C_2H, MgO, and $MgSiO_3$. For all these materials, we provide the pressure and internal energy over a wide density-temperature range from ~0.5 to 50 g/cc and from ~10^4 to 10^9 K. This database encompasses the results from approximately 5000 different first-principles simulations. It allows one to compute isobars, adiabats, and shock Hugoniot curves in the regime of L and K shell ionization. Invoking the linear mixing approximation, one can study the properties of user-defined mixtures at high density and temperature.

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(2) Start the *./fpeos* executable without arguments and go over the printed instructions

```
##############################################################################
#                                                                            #
# First-Principles Equation of State Database for Warm Dense Matter Computation #
#                                                                            #
# Burkhard Militzer                                    Berkeley, CA, 02-12-22  #
#                                                                            #
##############################################################################
```

(3) Pick any of the 21 compounds in the database and compute the shock Hugoniot curve for that material by executing a command like these

```
./fpeos EOS=2
./fpeos EOS=13
./fpeos EOS=21
```

In typical Unix fashion, execute “ls -ltr” to find out which files have been written most recently. You should see data files *.txt and graphics files *.pdf and *.png like shown here

```
  9108 May 19 09:35:28 2024 FPEOS_convex_hull.txt
329790 May 19 09:35:29 2024 FPEOS_isobars.txt
 92130 May 19 09:35:29 2024 FPEOS_isochor_points.txt
734562 May 19 09:35:30 2024 FPEOS_isochores_ideal_Debye.txt
740082 May 19 09:35:30 2024 FPEOS_isotherms.txt
 27992 May 19 09:35:30 2024 FPEOS_isotherm_points.txt
797425 May 19 09:35:32 2024 FPEOS_adiabats.txt
 48165 May 19 09:35:32 2024 FPEOS_Hugoniot.txt
 42465 May 19 09:35:32 2024 FPEOS_Hugoniot_lower_initial_density.txt
 54720 May 19 09:35:32 2024 FPEOS_Hugoniot_higher_initial_density.txt
 48165 May 19 09:35:33 2024 FPEOS_Hugoniot_rel.txt
 48578 May 19 09:35:33 2024 FPEOS_Hugoniot_rad.txt
 26188 May 19 09:35:36 2024 FPEOS_T_P_Debye_plot03.pdf
256800 May 19 09:35:37 2024 FPEOS_T_P_Debye_plot03.png
 26053 May 19 09:35:39 2024 FPEOS_T_E_Debye_plot03.pdf
279966 May 19 09:35:40 2024 FPEOS_T_E_Debye_plot03.png
 34683 May 19 09:35:42 2024 FPEOS_T_P_Ideal_plot03.pdf
395420 May 19 09:35:43 2024 FPEOS_T_P_Ideal_plot03.png
```

```
 33318 May 19 09:35:46 2024 FPEOS_T_E_Ideal_plot03.pdf
341713 May 19 09:35:47 2024 FPEOS_T_E_Ideal_plot03.png
 30944 May 19 09:35:49 2024 FPEOS_P_T_plot03.pdf
453798 May 19 09:35:50 2024 FPEOS_P_T_plot03.png
 37301 May 19 09:35:52 2024 FPEOS_rho_T_plot03.pdf
449769 May 19 09:35:53 2024 FPEOS_rho_T_plot03.png
 32046 May 19 09:35:56 2024 FPEOS_comp_T_plot03.pdf
425363 May 19 09:35:56 2024 FPEOS_comp_T_plot03.png
 44262 May 19 09:35:59 2024 FPEOS_comp_P_plot04.pdf
410302 May 19 09:36:00 2024 FPEOS_comp_P_plot04.png
 19980 May 19 09:36:02 2024 FPEOS_up_us_plot01.pdf
229121 May 19 09:36:03 2024 FPEOS_up_us_plot01.png
```

(4) Open the main shock Hugoniot file `FPEOS_Hugoniot.txt` and familiar yourself with the different columns that illustrate the thermodynamic conditions of the final shock states. With your favorite plotting software, plot the shock compression ratio, ρ/ρ_0, as function of temperature and then also as function of shock pressure. Do your plots look similar to any of the graphics files that were written by the *./fpeos* executable?

(5) In the file `FPEOS_Hugoniot.txt` find the conditions for the maximum value of the shock compression, which is typically between 4.3 and 5.5. Let's assume you have access to a laboratory with a gas gun that can generate shock waves with particle velocities (up in column 24) of up to 20 km/s but not more. What are the highest pressure and temperature that you can generate with your gas gun? Will you be able to reach the state of maximum compression for your chosen material?

(6) With diamond anvil cells, one is able to increase the initial density of shock experiments, ρ_0. If no arguments are specified, the database picks a default value for ρ_0. Look up the value in the file "FPEOS_Hugoniot.txt". Then increase and decreases the value in steps of approximately 20%. Execute "./fpeos rho0=..." for different density arguments and copy the resulting "FPEOS_Hugoniot.txt" file into a new file every time. Then compare the different Hugoniot curves in ρ/ρ_0-T and ρ/ρ_0-P spaces. How do the points of maximum compression shift as function of rho0?

(7) Invoking the ideal mixing approximation, let's study a material that is not directly contained in the database. For acetic acid $C_2O_2H_4$, execute

./fpeos binaryMixture EOS1=6 2.0 EOS2=16 2.0 rho0=1.049 E0=-229.0

and determine again which files have been written most recently.

(8) The compound H_2O and H_2O_2 are not in the database but one can again invoke the linear mixing approximation to derive the shock Hugoniot curve and expect the prediction to be reasonable accurate at high temperature like 2×10^5 K and sufficient high compression $\rho/\rho_0 \geq 3.2$. (see DOI: 10.1063/5.0023232)

./fpeos binaryMixture EOS1=1 2.0 EOS2=6 1.0 rho0=1.0 E0=-76.392172

./fpeos binaryMixture EOS1=1 2.0 EOS2=6 2.0 rho0=1.71330 E0=-151.489322

In each case one must look up the initial density in the experiment and derive the initial internal energy. This typically requires an all-electron DFT calculation.

(9) We can probe the accuracy of the ideal mixing approximation by comparing the calculations.

a) Compute the shock Hugoniot curve of CH plastic with "./fpeos ..." Look up the values for E_0 and ρ_0. (Multiply E_0 by -1 because it is not printed with the correct sign. Sorry!)

b) Compute the same Hugoniot curve by assuming an ideal mixture of carbon and hydrogen with

./fpeos binaryMixture EOS1=... 1.0 EOS2=... 1.0 rho0=... E0=...

Compare the predictions in the files "FPEOS_Hugoniot.txt" and "FPEOS_mixture_Hugoniot.txt" by plotting the two Hugoniot curves in ρ/ρ_0-T and ρ/ρ_0-P spaces. How big is the error of the ideal mixing approximation at the point of maximum compression?

(10) Finally we want to probe the accuracy of the ideal mixing for $MgSiO_3$, which is contained in the database. So first calculate its shock Hugoniot curve with

./fpeos EOS=...

and look up the density and initial internal energy E_0 and ρ_0 in the shock Hugoniot file. Then compute the Hugoniot curve invoking the ideal mixing approximation:

./fpeos ternaryMixture EOS1=... 1.0 EOS2=... 1.0 EOS3=... 3.0 rho0=... E0=...

And compare the two Hugoniot curves.

Well done! Thank you for completing this tutorial. Please let me know what challenges you encountered along the way so that it can be improved for the future. Thank you very much!