Fundamentals of SESAME Equation of State

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Equation of State

What is an Equation of State anyway?

- An equation of state is a set of thermodynamic functions for a given material.
  - Partial EOS
    - Ideal gas
    - Virial expansion
    - Steinberg
  - Complete EOS
    - most easily defined using thermodynamic potentials

Equation of State

Breadth of Problems

- Wide Variety of Complex Materials
  - Actinides (Pu, U, etc.)
  - Elemental Metals
  - Alloys and Chemical Compounds
  - Molecular Solids and Liquids
  - Polymers, Foams, Composites, and Geological
  - High Explosives
- Ambient to Astrophysical Conditions ($10^{-6} < \rho/\rho_o < 10^5$, $0 < T < 10^5$eV)
- Nonequilibrium Processes (melting & refreezing)
- Large Ranges of Interpolation Between Models
- Incomplete Experimental Information

Solutions

- More Basic Theory
- Improved Modeling
- Increased Support of Experiments

So…..What about high pressure?

P (Mbar)	
0.000001	Ambient
1	Center of Earth
100	Center of Jupiter
340	Insulating Nickel
> 1340	Metallic Neon
350000	Center of Sun
100000000	Highest P_c for Al in SESAME

Specifics of SESAME EOS

- ✓ Our thermodynamic potential is Helmholtz free energy:

$$F(\rho,T) \quad \text{or} \quad A(\rho,T)$$

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Specifics of SESAME EOS

- We define all extrinsic quantities (energy, entropy, etc.) per unit mass

$$V=1/\rho$$

- Units:

ρ	*g/cm³*	
T	*K*	*(ev)*
E	*MJ/kg*	*(Mbar cm³/g)*
P	*GPa*	*(Mbar)*
velocity	*km/s*	*(cm/μs)*

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Three-term decomposition of EOS

- ✓ We express the Helmholtz free energy as:

$$F(V,T) = \phi_0(V) + F_{\text{ion}}(V,T) + F_{\text{el}}(V,T)$$

$\phi_0(V)$	cold curve contribution
$F_{\text{ion}}(V,T)$	cold + thermal ionic contribution
$F_{\text{el}}(V,T)$	thermal electronic contribution

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Basic thermodynamic quantities

$$E = F + TS = F - T\left(\frac{\partial F}{\partial T}\right)_V \longleftarrow$$ Internal energy

$$S = -\left(\frac{\partial F}{\partial T}\right)_V \longleftarrow$$ Entropy

$$P = \rho^2\left(\frac{\partial F}{\partial \rho}\right)_T \longleftarrow$$ Pressure

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Basic thermodynamic quantities

$$C_V = -T\left(\frac{\partial^2 F}{\partial T^2}\right)_V = \left(\frac{\partial E}{\partial T}\right)_V = T\left(\frac{\partial S}{\partial T}\right)_V \longleftarrow$$ Specific heat at constant volume

$$C_P = \left(\frac{\partial H}{\partial T}\right)_P = T\left(\frac{\partial S}{\partial T}\right)_P \longleftarrow$$ Specific heat at constant pressure

$$B_T = V\left(\frac{\partial^2 F}{\partial V^2}\right)_T = -V\left(\frac{\partial P}{\partial V}\right)_T \longleftarrow$$ Isothermal bulk modulus

$$B_S = -V\left(\frac{\partial P}{\partial V}\right)_S \longleftarrow$$ Adiabatic bulk modulus

$$\frac{B_S}{B_T} = \frac{C_P}{C_V}$$

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Basic thermodynamic quantities

$$\alpha = -\frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_P \longleftarrow$$ Thermal expansion coefficient

$$\gamma = V\left(\frac{\partial P}{\partial E}\right)_V = \frac{\alpha V B_T}{C_V} \longleftarrow$$ Gruneisen parameter

SESAME Database

- ✓ Origins of the database
- ✓ Basic elements

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SESAME Database

1949 -- Feynman, Metropolis, and Teller

"Equations of State of Elements Based on the Generalized Fermi-Thomas Theory"

1956 -- Cowan and Ashkin

TFD

-- Cowan

"self-contained form for the ionic EOS"

1971 -- Jack Barnes and Jerry Kerley

The SESAME database was created

1972 -- The library first became publicly available

SESAME Distribution

SESAME has a wide user base it has been distributed to:

- Foreign Countries
- US Government
- US Corporations
- US Universities
- Internal LANL Divisions

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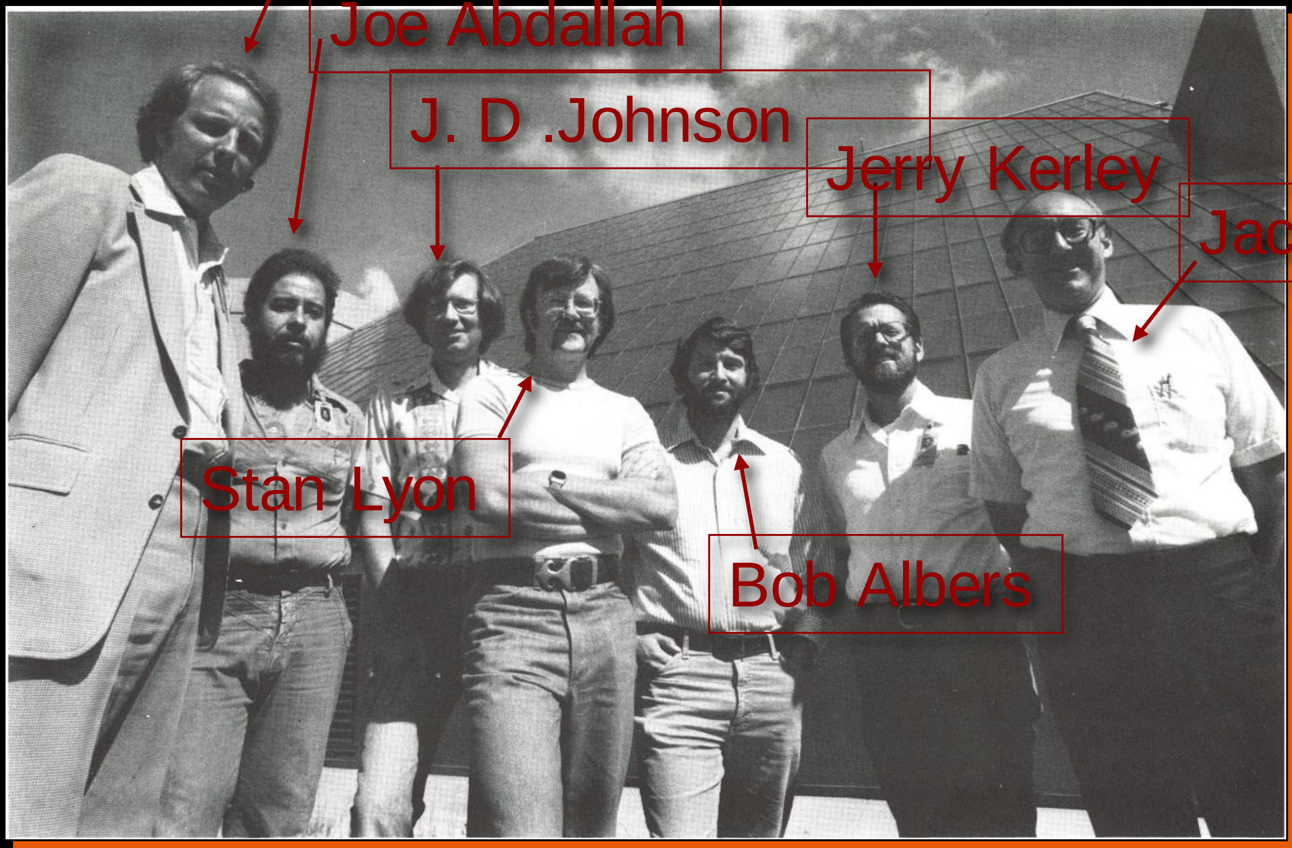
Class of 1979



The SESAME database structure

- Library → Material → Table → Data
- Materials are Indicated by numbers (material IDs)
  - Numbering conventions
    - EOS (0-9999, 50000, 90000 for beta/experimental only)
    - Opacity (10000 or 60000)
    - Conductivity (20000 or 70000)
    - Melt and Shear tables (30000 or 80000)

The SESAME library table/data types

- 100 series -- comments
  - 101 -- fixed form with basic information (name etc.)
  - 102-199 (all others) -- free-form text describing anything else
- 201 atomic number, atomic weight, reference density, etc.
- 300 series stores functions on a density-temperature grid
  - 301 -- total ρ, T, P, E, A
  - 303 -- cold + nuclear
  - 304 -- electronic
  - 305 -- nuclear
  - 306 -- cold ρ, T, P, E, A (= E)
  - 311 -- Maxwell constructed 301 (internal only)
  - 321 -- mass fractions for multiphase EOS

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The SESAME library table/data types

- 400 series stores functions along a curve
  - 401 -- vapor dome ρ, T, P, E, A
  - 411 -- solidus ρ, T, P, E, A
  - 412 -- liquidus ρ, T, P, E, A
  - 431 -- shear modulus at T=0
  - 432 -- shear modulus at T=0 and $T=T_M$
- 500 series -- opacity
- 600 series -- conductivity

The SESAME library table/data types

- Data formats
  - binary file (SESAME)-- used in all Laboratory applications
  - ascii file -- used in most external applications
    - CTH, Mach2, Autodyn, Helios
  - directory structure -- used by OpenSesame
  - XML -- next generation library

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The SESAME ascii file

```
 0  3720   101   240   r    82803    22704   1                               0
material. aluminum (z=13.0, a=26.9815) /source. S. D. Crockett, T-1/date. Aug.28
  /refs. LAUR-04-6442 /comp. Al /codes. GRIZZLY (ver. 030603)  /Classification.
Unclassified /
 1  3720   102   320   r    82803    22704   1                               1
This EOS was produced to using the standard LANL GRIZZLY models. The aluminum EO
S is an improvement over prior SESAME EOS produced.  A comparison to the 3710 se
ries is provided in LAUR-04-6442. A copy of all the input decks required to repr
oduce this EOS are contained in the above report.
 1  3720   201     5   r    82803    22704   1                               1
 1.300000000000000E+01 2.698150000000000E+01 2.700000000000000E+00 0.000000000000000E+00 0.000000000000000E+0011111
 1  3720   301 26165   r    82803    22704   1                               1
 1.110000000000000E+02 7.800000000000000E+01 0.000000000000000E+00 2.700000000000000E-06 5.400000000000000E-0611111
 1.350000000000000E-05 2.700000000000000E-05 5.400000000000000E-05 1.350000000000000E-04 2.700000000000001E-0411111
 5.400000000000001E-04 1.350000000000000E-03 2.700000000000000E-03 4.050000000000001E-03 6.750000000000000E-0311111
 1.080000000000000E-02 1.620000000000000E-02 2.700000000000000E-02 4.050000000000001E-02 6.750000000000000E-0211111
 1.080000000000000E-01 1.620000000000000E-01 2.160000000000000E-01 2.700000000000000E-01 3.375000000000000E-0111111
 4.050000000000001E-01 ……………..……..……..……..….
```