Issues in Equation of State data generation for Hot Dense Matter
A Note on Generalized Radial Mesh Generation for Plasma Electronic Structure

B. G. Wilson, V. Sonnad

February 17, 2011

High Energy Density Physics
Disclaimer

This document was prepared as an account of work sponsored by an agency of the United States government. Neither the United States government nor Lawrence Livermore National Security, LLC, nor any of their employees makes any warranty, expressed or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States government or Lawrence Livermore National Security, LLC. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States government or Lawrence Livermore National Security, LLC, and shall not be used for advertising or product endorsement purposes.
Abstract
Precise electronic structure calculations of ions in plasmas benefit from optimized numerical radial meshes. A new closed form expression for obtaining non-linear parameters for the efficient generation of analytic log-linear radial meshes is presented.

1. Introduction
Radial grids for the numerical solution of electronic wavefunctions are usually based on a transformation of an evenly spaced auxiliary variable. This allows convenient numerical approximations to solutions of the governing Dirac differential equation and matrix element quadratures. The transformation is prototypically an exponential mapping

\[ r_k = r_c e^{kh} \quad k = 1,2,... \]

that preferentially places radial points near the origin where atomic potentials are varying rapidly. However for continuum wave-functions or plasma and solid state cellular calculations, where the large radial mesh spacing is too coarse to adequately describe variations near the outer boundary, a variant log-linear radial mesh, defined by the implicit equation

\[ kh = \alpha \frac{r_k}{r_c} + \log \left[ \frac{r_k}{r_c} \right] \]

is of greater utility. The parameter ‘\( \alpha \)’ analytically modifies the grid from a pure exponential mesh near the origin to a mesh that has linear spacing asymptotically.

For an ‘\( N \)’ point mesh, given physically motivated values for the first radial mesh point ‘\( r_1 \)’ (typically a small value \( r \approx 6.25x10^{-5} \) Bohr is adequate for even heavy elements) and ‘\( r_N \)’ (e.g. the plasma ion sphere radius) there is a continuum of parameterizations \( h(\alpha), r_c(\alpha) \), non-linear in \( \alpha \), that describes a radial mesh that evolves from pure logarithmic spacing to near linear spacing at the outer boundary. This note presents a novel closed form relation for \( h(\alpha), r_c(\alpha) \).

2. Method
The implicit equation for the radial mesh generation can be conveniently reformulated in the explicit form

\[ r_k = r_c e^{kh} \left[ \alpha e^{kh} \right] \]

by introducing
\[ \omega[x] = \frac{W[x]}{x} \]

where W[x] is Lambert’s function \[i\], which is defined implicitly by
\[ x = We^W \]

We note that \( \omega[0] = 1 \), that \( \omega[x] \) is a monotonically decreasing function of \( x \), and that \( \omega \), \( W \) and their logarithms can be evaluated directly by a simple, rapidly convergent iteration algorithm \[ii\]. Formally, for a given parameter ‘\( \alpha \)’ the value of ‘\( h \)’ is determined by that of the first radial mesh point and the value ‘\( r_n \)’ at the last index ‘\( n \)’, by the implicit equation
\[
\log \left( \frac{r_n}{r_1} \right) = (n-1)h + \log \left( \frac{\omega[\alpha e^{nh}]}{\omega[\alpha e^h]} \right)
\]
The value of ‘\( r_c \)’ then follows directly from the value of ‘\( h \)’ via
\[ r_c = \frac{r_1}{e^{h_0} \omega[\alpha e^h]} \]

The assumed value of ‘\( \alpha \)’ is a consequence of further considerations on the desired properties of the radial mesh. For example: that the outermost mesh spacing does not exceed a specified value or that there be a specified number of points in an outer portion of the radial mesh. In general the value of ‘\( \alpha \)’ must be numerically determined iteratively in conjunction with obtaining values of ‘\( h \)’ and ‘\( r_c \)’ as a non-linear function of ‘\( \alpha \)’. In practice this non-linear self-consistency takes unwarranted cpu time.

The central result of this note is that the implicit equation for \( h[\alpha] \) has a remarkable closed form solution:
\[
h = h_0 - \left( \frac{d}{s} \right) W[-\alpha s]
\]

where
\[
h_0 \equiv h[\alpha = 0] = \frac{1}{(n-1)} \log \left( \frac{r_n}{r_1} \right)
\]

The parameter
\[ d \equiv e^{h_0} - e^{h_0} \]
\[ (n-1) \]
is positive definite for all \( h_0 > 0 \) while
\[ s \equiv \frac{e^{nh_0} - ne^{h_0}}{(n-1)} \]
is positive if (and only if) \( r_n > nr_1 \). We note that Lambert’s function \( W[x] \) is real and single valued only for values of argument \( x > -e^{-1} \); this places an upper limit to the allowed value of ‘\( \alpha \)’ for a given value of \( r_i \) and \( r_n \).

The author is unaware of any direct proof of the above identity. It was obtained by re-summing the Taylor expansion of \( h[\alpha] \) using high order coefficients obtained by analytic differentiation of the implicit definition using MATHEMATICA symbolic manipulation.

3. Summary

In conjunction with the (very simple) algorithm for the rapid high precision evaluation of Lambert’s W-function, the above identity allows the precise construction of generalized log-linear radial meshes adapted to various constraints.

Acknowledgments

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

\[ ^i \] Implemented in MATHEMATICA as the function “ProductLog[x]”.
\[ ^{ii} \] F. Fritsch, Commun. ACM 16, p.123 (1973)