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

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High Energy Density Physics

Disclaimer

A Note on Generalized Radial Mesh Generation for Plasma Electronic Structure

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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

$$r_k = r_c e^{kh} \qquad k = 1,2,...$$

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 'α' 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 $r_1 \cong 6.25x10^{-5}$ 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 α, 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

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

by introducing

$$\omega[x] \equiv \frac{W[x]}{x}$$

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 ω, W and their logarithms can be evaluated directly by a simple, rapidly convergent iteration algorithm [ii]. Formally, for a given parameter 'α' 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

$$Log\left[\frac{r_n}{r_1}\right] = (n-1)h + Log\left[\frac{\omega\left[\alpha e^{nh}\right]}{\omega\left[\alpha e^{h}\right]}\right]$$

The value of 'r_c' then follows directly from the value of 'h' via

$$r_c = \frac{r_1}{e^h \omega\left[\alpha e^h\right]}$$

The assumed value of 'α'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 'α'must be numerically determined iteratively in conjunction with obtaining values of 'h' and 'r_c' as a non-linear function of 'α'. In practice this non-linear self-consistency takes unwarranted cpu time.

The central result of this note is that the implicit equation for h[α] has a remarkable closed form solution:

$$h = h_0 - \left(\frac{d}{s}\right) W\left[-\alpha s\right]$$

where

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

The parameter

$$d \equiv \frac{e^{nh_0} - e^{h_0}}{(n-1)}$$

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) $r_n > n\,r_1$. 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 'α' for a given value of r_1 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[α] 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.

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[i] Implemented in MATHEMATICA as the function "ProductLog[x]".

[ii] F. Fritsch, Commun. ACM 16, p.123 (1973)