A COMPARISON OF VARIOUS NLTE CODES IN COMPUTING THE CHARGE-STATE POPULATIONS OF AN ARGON PLASMA

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A comparison among nine computer codes shows surprisingly large differences where it had been believed that the computational physics was well understood. The codes simulate a plasma that is in steady state but not in local thermodynamic equilibrium (NLTE codes). In this study each code treats an "easy" problem, which is an argon plasma, optically thin and with no external photon flux; densities are varied from near-coronal to an intermediate 10^{21} electrons/cc and above. The temperatures are high enough that most ions have two or fewer bound electrons, which for this plasma means temperatures above about 300 eV.

The present study asks only if the codes compute similar charge-state populations (a surprising "no"), and, if not, why not. It does not claim accuracy for any code either by comparison to experiment or by appeal to a concensus.

A striking feature of the ionic populations computed by the various codes is their dissimilarity: The agreement varies from near exact to more than 2.5 orders of magnitude different, and if we ignore extremes, still the typical disagreement is about a factor of 2.

We seek clues to why the codes disagree by modifying bits of physics within a single code. What happens to the charge-state populations in the Ar plasma if a rate coefficient is arbitrarily cut in half or if the allowed number of excited states is reduced? It is found that populations computed by a single code vary by about a factor of 2 if

(i) electron-collisional excitation/de-excitation is cut in half; or
(ii) electron-collisional ionization/recombination is cut in half; or
(iii) the maximum principal quantum number n_{max} is reduced from 12 (allowed by continuum lowering) to only 5. See Figure 1.

The computed populations seem most at risk from n_{max} being set too small. This is because rate coefficients are computed with care (especially for H- and He-like ions), while continuum lowering and n_{max} are often set arbitrarily. For instance, we note that four formulae often used for e-collisional ionization/recombination vary by some 15% or less in the Ar problem. On the other hand, most codes do not compute n_{max} but fix it *a priori*.

Results of this study are being compiled in a LLNL internal report due to become available in the autumn of 1984.

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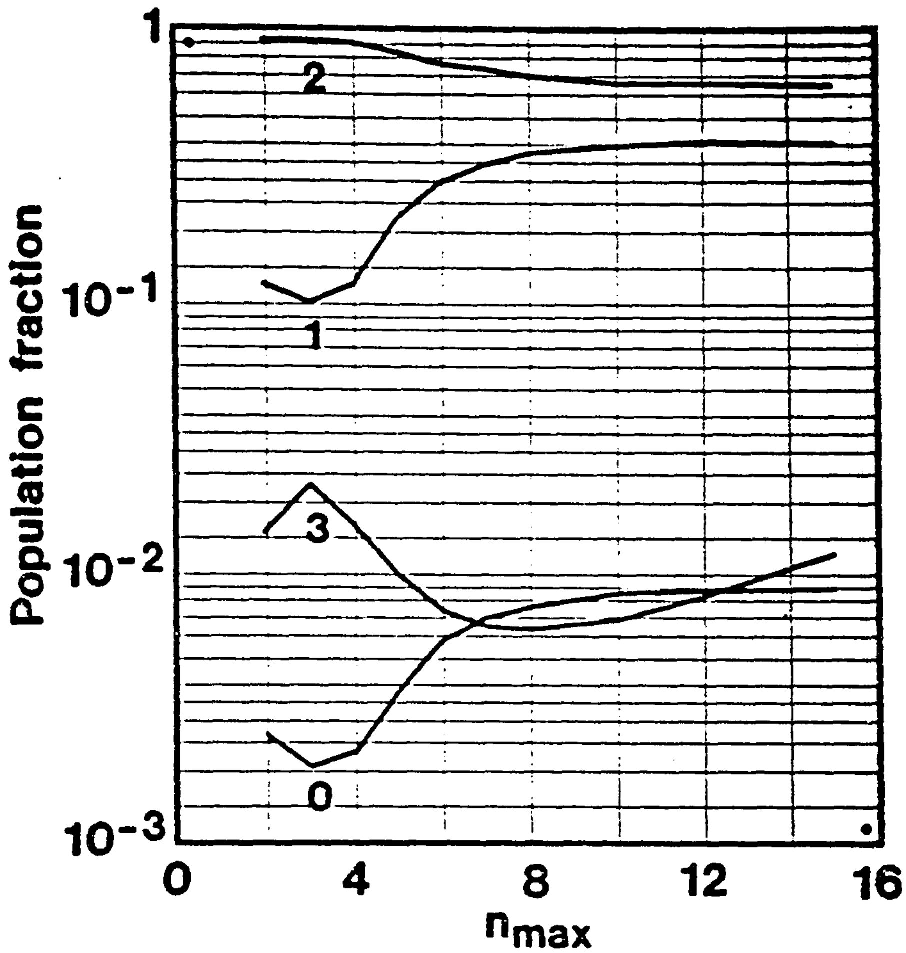
Figure 1: Effect of n_{max} on populations. The code LINEZ computes the population fraction of charge-states with 0, 1, 2, and 3 bound electrons. The plasma is argon, optically thin, with particle temperature 1 keV and a density of 5.6×10^{19} ions/cc. For this figure LINEZ lowers the continuum by the Stewart-Pyatt algorithm, then fixes the maximum allowed principal quantum number at n_{max} for each ionic charge-state.



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