Comparison of Simulation Software

EUROSIM - Simulation News Europe started a series on comparisons of simulation software. Based on simple, easily comprehensible models special features of modelling and experimentation within simulation languages, also with respect to an application area, shall be compared.

The idea has become quite successful. Here we would like to thank all the authors who took the challenge and the time, solved the problems, documented them and sent in their contributions.

Up to now each issue of EUROSIM - Simulation News Europe introduced a new comparison. We now repeat the description of the first two comparisons so that you can still participate, especially with simulation languages that have not yet been introduced. Also a new comparison is published, page 31.

We invite all institutes and companies developing or distributing simulation software to participate in this comparison:

Please, simulate the model described and send a report to the editors in the following form:

- short description of the language
- model description (source code, diagram, ...)
- results of the tasks with experimentation comments
- approx. 1 page A4

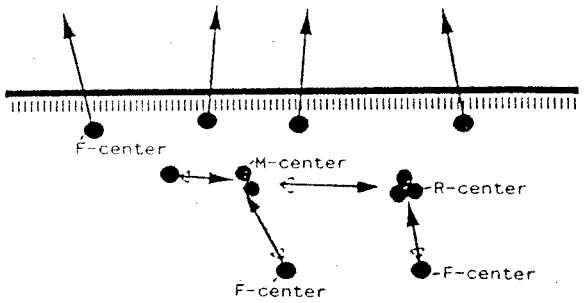
Reports will be published in the next issues of EUROSIM - Simulation News Europe.

New comparisons will be prepared for the next issues. As it is difficult to find suitable "simple" models and relevant tasks we would like to ask you to contact the editors if you have an idea for a model to be compared in different simulation languages.

Comparison 1: Lithium-Cluster Dynamics under Electron Bombardment

The first model to be compared is taken from solid state physics. The special features to be compared are rate equations (application area), stiff systems (numerical integration), parameter sweep and steady-state calculation (experimentation).

The model describes formation and decay of defect ("F-centers") aggregates in alcali halides. The defects are produced by electron bombardment near the surface of the crystal and can either form aggregates or will evaporate if they reach the surface.



The variable f(t) denotes the concentration of F-centers, m(t) and r(t) respectively denote the concentration of aggregates consisting of two (M-center) or three F-centers (R-center). In principle the system can be easily extended taking into account formation of larger aggregates (n F-centers). The variable p(t) is the production term of F-centers due to electron bombardement (irridiation):

$$dr/dt = -d_r r + k_r mf$$
$$dm/dt = d_r r - d_m m + k_f f^2 - k_r mf$$
$$df/dt = d_r r + 2d_m m - k_r mf - 2k_f f^2 - l_f f + p$$

The parameter l_f measures the loss of F-centers at the surface. k_r and k_f are rate constants describing the formation of an M-center out of two F-centers, or the formation of an R-center out of an M-center and an F-center. The decay of an R-center into an M-center and an F-center is described by the rate constant d_r and the decay of an M-center into two F-centers by the rate constant d_m. Investigations are started after constant electron bombardment $p(t) = p_c = 10^4$ of approximately 10 s; the production term has to be set to zero ($p(t) = 0$), the initial values are:

$$f(0) = 9.975$$
$$m(0) = 1.674$$
$$r(0) = 84{,}99$$

The parameter values are:

$$k_r = 1$$
$$k_f = 0.1$$
$$l_f = 1000$$
$$d_r = 0.1$$
$$d_m = 1$$

The following tasks should be performed

a) simulation of the stiff system over [0,10] with indication of computing time depending on different integration algorithms.

b) parameter variation of l_f from 1.0E2 to 1.0E4 and a plot of all $f(t;l_f)$, logarithmic steps preferred.

c) calculation of steady states during constant bombardment $p(t) = p_c = 1.0E4$) and without bombardment ($p(t) = 0$).

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