PACKAGE ID - 000238IBMPC03 SIMION3D7.0REV

KWIC TITLE - Models Ion Trajectories in 2D and 3D Electrostatic and Magnetic Fields

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LIMITATION CODE -COPY **AUDIENCE CODE -** LIM

COMPLETION DATE - 02/01/2000 **PUBLICATION DATE -** 02/01/2000

DESCRIPTION - SIMION3D7.0REV is a C based ion optics simulation program that can model complex problems using Laplace equation solutions for potential fields. The program uses an ion optics workbench that can hold up to 200 2D and/or 3D electrostatic/magnetic potential arrays. Arrays can have up to 50,000,000 points. SIMION3D7.0's 32 bit virtual Graphics User Interface provides a highly interactive advanced user environment. All potential arrays are visualized as 3D objects that the user can cut away to inspect ion trajectories and potential energy surfaces. User programs allow the user to customize the program for specific simulations. A geometry file option supports the definition of highly complex array geometry. Algorithm modifications have improved this version's computational speed and accuracy.

PACKAGE CONTENTS - Media Directory; Software Abstract; Media Includes Source Code, User's Guide, Executable Module, Auxiliary Material, Compilation Instructions, Linking Instructions, User's Demos;

SOURCE CODE INCLUDED? - Yes

MEDIA QUANTITY - 1 CD Rom

METHOD OF SOLUTION - Electrostatic and Magnetic fields are determined by numerically solving the Laplace equation via finite difference techniques. These techniques make use of over-relaxation and skipped point refining techniques to obtain solution times that are proportional to n (where n is the number of points in the array). A highly modified Runge-Kutta method is used to calculate ion trajectories in these fields. Automatically self-adjusting time steps make use of curvature and edge detection along with binary boundary approach methods to minimize the number of integration steps required to maintain ion trajectory accuracy.

COMPUTER - IBM PC

OPERATING SYSTEMS - Win32 application in Windows 9x, NT, and 2000

PROGRAMMING LANGUAGES - C (100%)

SOFTWARE LIMITATIONS - Each array point takes 10 bytes. Thus a 1,000,000 point array requires 10 MB of RAM or virtual RAM.

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SOFTWARE LIMITATIONS -(CONT) Maximum array size: 50,000,000 points. maximum number of arrays in workbench: 200. Maximum workbench size: Plus or minus a cubic kilometer.

SOURCE CODE AVAILABLE (Y/N) - Y

UNIQUE FEATURES - The program allows the modeling and visualization of complex ion optics systems on widely available Intel based personal computers. Its most unique features are its breadth of power and easy-to-use visual graphics user interface.

RELATED SOFTWARE - SIMION3D7.0REV supersedes all previous SIMION versions.

OTHER PROG/OPER SYS INFO - Potential arrays have .PA extensions. Program provided in executable format. Source code is provided without support for those who need to modify the program.

HARDWARE REQS - The program requires the following: A math coprocessor, at least 16MB of RAM, a Windows screen resolution of 800 x 600 x 256 colors or better, and a printer that is supported by Windows or uses one of the following languages: PostScript, PCL5, HGPL2, or HPGL.

TIME REQUIREMENTS - The refining of 16,000 point arrays takes about 10 seconds on a 486DX2 66MHz personal computer. Typical 3D view visualizations take from 1 to 10 seconds. A single ion flight can take one or more seconds depending on what is being modeled.

REFERENCES - David A. Dahl, SIMION 3D Version 76.0 User's Maual, INEL-95-0403 Rev. 5, February 2000.

ABSTRACT STATUS - Released AS-IS 8/16/2000

SUBJECT CLASS CODE - TW

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DATA

EDB SUBJECT CATEGORIES -
990200

SPONSOR - DOE/ER

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