

PACKAGE ID - 001215MLTPL00 MPSALSA

KWIC TITLE - Chemically Reacting Flows Modeler

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

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DESCRIPTION - MPSALSA solves the governing equations for chemically reacting flows, as appropriate for simulating systems such as Chemical Vapor Deposition reactors. Transport equations for incompressible flow, heat transfer, and mass transfer with chemical reactions in two and three dimensions are solved simultaneously. Efficient and robust algorithms for performing these calculations on massively parallel computers are used.

PACKAGE CONTENTS - Media Directory; Software Abstract; SAND95-2752; SAND96-2331; Media Includes Source Code, Object Library, Executable Module, Sample Problem Input and Output Data;

SOURCE CODE INCLUDED? - Yes

MEDIA QUANTITY - 1 CD Rom

METHOD OF SOLUTION - An unstructured grid finite element method is used to solve the governing equations of fluid flow, heat transfer, and mass transfer. A fully-coupled Newton method is used to solve for steady-state solutions or for implicit time integration. The parallel implementation of these methods includes explicit message passing between processors, and allows for the solution of meshes on the order of a million elements.

COMPUTER - MLT-PLTFM

OPERATING SYSTEMS - UNIX, SUNMOS, COUGAR

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PROGRAMMING LANGUAGES - C (99%) FORTRAN (1%)

SOFTWARE LIMITATIONS - Requires as input finite element mesh in ExodusII format. Parallel computations require MPI library except on Intel machines.

SOURCE CODE AVAILABLE (Y/N) - Y

UNIQUE FEATURES - MPSALSA solves the governing equations on unstructured grids, which allows for modeling of complex geometries, and solves them using parallel processors, so that very large problems can be solved in a reasonable amount of time. The equations are solved fully-coupled, which greatly improves convergence behavior over other methods.

RELATED SOFTWARE - Aztec, Chaco, SEAMS distribution (fastq, blot, exolexo2v2, ExodusII library, netcdf library), Chemkin, ARPACK, gmake.

OTHER PROG/OPER SYS INFO - The user's guide gives details about running MPSALSA.

HARDWARE REQS - No requirements. The more memory available on the computer, the bigger the problem that can be run.

TIME REQUIREMENTS - The required time to run the code is completely dependent on the specific problem, in particular the number of equations to solve per node and the number of nodes in the mesh. A two-dimensional fluid flow problem on a few thousand element mesh should take about a minute to solve on a modern workstation.

REFERENCES - John N. Shadid, Harry K. Moffat, Scott A. Hutchinson, Gary L. Hennigan, Karen D Devine, and Andrew G. Salinger, MPSALSA A Finite Element Computer Program for Reacting Flow Problems, Part 1 Theoretical Development, SAND95-2752, May 1996; A. Salinger, K. Devine, G. Henningan, H. Moffat, S. Hutchinson, and J. Shadid, MPSALSA A Finite Element Computer Program for Reacting Flow Problems, Part 2 User's Guide, SAND96-2331, Septmeber 1996.

ABSTRACT STATUS - Released AS-IS 5/5/1998.

SUBJECT CLASS CODE - H

KEYWORDS -

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M CODES
FINITE ELEMENT METHOD
FLUID FLOW
HEAT TRANSFER
COMPUTERIZED SIMULATION
STEADY-STATE CONDITIONS

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SOFTWARE ABSTRACT

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EDB SUBJECT CATEGORIES -
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