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COMPUTATIONAL INVESTIGATION OF A MODEL LINKING ALGORITHM FOR THE ENERGY-ECONOMY INTERACTION MODEL

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Scope and Purpose—Energy economy interaction analyses are increasingly important to policy makers and researchers under increasing import energy prices. Conventionally, macroeconomic indices are assumed given, so that energy sector analysis is carried out in a partial equilibrium framework. Since some of major economic variables have been observed to vary through feedback effects due to major changes in energy sector, energy-economy linkage schemes have recently received increasing attention within the research and policy making communities.

This linkage could, however, create computational difficulties to simulate this combined, possibly large-scale, integrated system. Furthermore, this linkage or integration might ask for sacrifice on the part of component models (energy sector submodel or macroeconomic submodel) in terms of independent modularity. In this regard, it is highly desirable to develop and apply a computational scheme which utilizes component submodels as they are, but could find or generate a solution or equilibrium point of the integrated system. Typically, this type of approaches are subject to convergence issues, in particular when some of component submodels are of process analysis type (or linear programming type). This paper tries to answer this set of issues.

Abstract—A model linking algorithm which is based on the algorithmic concept employed in the Project Independence Evaluation System (PIES) is developed for a dynamic energy/economic interaction model. The convergence of the algorithm is tested empirically and the results show that the algorithm converges to the desired accuracy. Potential application to generalized networks is discussed.

Results of this work confirms the possibility of utilizing the PIES algorithm concept as a model integration scheme in general network situations.

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INTERACTIVE MODELING OF ENZYME-INHIBITOR COMPLEXES AT MERCK MACROMOLECULAR MODELING GRAPHICS FACILITY†

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Abstract—Merck Sharp & Dohme Research Laboratories has developed enzyme-inhibitor modeling procedures based on the convenient display and manipulation features of the FRODO crystallographic modeling program (Jones, 1978, 1982). After implementing the program on a VAX computer controlling an Evans & Sutherland Multi Picture System, we have added useful techniques such as multiple superpositions, color-coded labels and dot surfaces, and a novel real-time atomic contact display ("CLARIFI") which emphasizes crucial repulsions while showing nonspecific binding.

A synthetic chemist in Merck's New Leads Discovery Department has used these tools to develop a revised picture of the transition state and substrate specificity of the zinc protease thermolysin (Hangauer *et al.*, 1983a). A movie illustrating the model was produced with the aid of GRAMPS (O'Donnell & Olson, 1981).

Our enzyme-inhibitor modeling also makes use of links to the existing small-molecule Merck Molecular Modeling System, and to empirical energetics programs. These techniques are complementary and should be seen as tools with which a scientist can generate and test structural ideas.