

MESHLESS STOCHASTIC SIMULATION OF MICRO-MACRO MODELS ARISING FROM KINETIC THEORY

*E. Cueto¹, M. Laso² and F. Chinesta³

¹ Aragón Institute of Engineering Research (I3A)
Universidad de Zaragoza
María de Luna s/n.
50018 Zaragoza, Spain.
e-mail: ecueto@unizar.es,
http://gemm.unizar.es

² Laboratory of Non-Metallic
Materials
Dept. of Chemical Engng.
Univ. Politécnica de Madrid
José Gutiérrez Abascal, 2
E-28006 Madrid, Spain

³ Laboratoire de Mécanique
des Systèmes et des Procédés
UMR CNRS-ENSAM-ESEM
151, boulevard de l'Hôpital,
75013 Paris, France

Key Words: *Kinetic theory, FENE model, reptation, meshless methods, updated Lagrangian.*

ABSTRACT

We present in this paper a numerical technique for the stochastic simulation of molecular models of visco-elastic fluids based on kinetic theory. The technique is based on the use of meshless methods (particularly, the Natural Element Method, NEM) and allows for an updated lagrangian description of the conservation equations.

In this way, model molecules are associated with nodal positions such that they are advected with material velocities. Problems associated with lack of molecules in certain elements, for instance, as encountered in the basic implementation of CONNFFESSIT approaches, are thus avoided. The technique is based on the use of Natural Neighbor Galerkin schemes, that allow for a proper geometrical description of the domain as it evolves. The presented technique is especially well suited for the numerical simulation of free-surface flows. We present examples of validation and also performance tests of this technique applied to FENE and reptation (Doi-Edwards) models.