Meeting: 1002, Pittsburgh, Pennsylvania, SS 7A, Special Session on Knots and Macromolecules

1002-65-182Michael Piatek* (piatek@mathcs.duq.edu), Duquesne University, Dept of Mathematics and
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Cantarella. Numerics issues in ropelength minimization.

Discovering ideal, or ropelength minimized knots and links is a difficult problem for direct analysis. Most often, approximate minimizers are computed using numerical methods. We will consider the often subtle numerical difficulties the authors have encountered when applying simulated annealing and the conjectured ropelength gradient to this problem. Approaches for controlling thickness and edge length will be considered, as well as the numerical difficulty of the minimum radius of curvature. These techniques may be applicable to future numerical algorithms in the area. (Received September 13, 2004)