Numerical analysis of non-equilibrium dynamics of polymeric liquid and solid

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We have developed two codes [1,2] implemented to massively parallel code, LAMMPS [3]. The one is for elongational flow successful in molecular dynamics simulation [1]. The other is multiscale simulation code coupling finite element method and molecular dynamics simulation [2].

Elongational flow was difficult on molecular dynamics simulation because the simulation box was collapsed within a finite simulation time. We can avoid this collapse if we set the initial simulation box not parallel to elongational direction. We have succeeded in obtaining the elongational viscosities on molecular dynamics simulation. The details are found in Ref [1].

Multiscale simulation coupling macroscopic continuum simulation and molecular dynamics simulation was difficult because the general deformation or strain was not dealt within the conventional technique on molecular dynamics simulation. The general strain can be decomposed to a rotation tensor and a stretch tensor by using QR decomposition. Using this technique, we have succeeded in coupling finite element method and molecular dynamics simulation and investigated a uniaxial loading of polymeric solid. The details are found in Ref [2].

References

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