

<b>Title</b>	Derivation of coarse-grained potential for polyethylene
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<b>Purpose of this study</b>	In this study, we propose a new method to derive a set of coarse-grained potentials for polyethylene.
<b>System (Material)</b>	Polyethylene
<b>Program (including analysis)</b>	COGNAC v1.2 spline smoothing
<b>Method &amp; Some important input parameters</b>	(Method) While the effective bonded potentials are determined by simply taking the logarithm of the corresponding distribution functions calculated from the microscopic simulations, the effective non-bonded potentials are evaluated using the canonical ensemble average for the fixed non-bonded distance. (Input) Number of atoms, NVT or NPT ensemble, temperature, pressure
<b>Advance &amp; Problem</b>	Advance: The coarse-grained model combined with the aforementioned effective potentials can reproduce the radii of gyration, the distribution functions of the coarse-grained variables and the densities.  Problem: We would require to take the correlation effects between bonded variables and between bonded and non-bonded variables.
<b>Reference</b>	[Manuscript] : Accepted Comput. Phys. Commun., in press [Presentation at conferences (Meetings)] Japan Molecular simulation conference 2000 Conference on Computational Physics 2000
<b>Keyword (in English)</b>	molecular dynamics (MD) simulation , Gay-Berne (GB) potential, Lennard-Jones (LJ) potential, OPLS potential, liquid crystal, nematic, nCB(4-n-alkyl-4'-cyanobiphenyl)

## Results (Remarks)

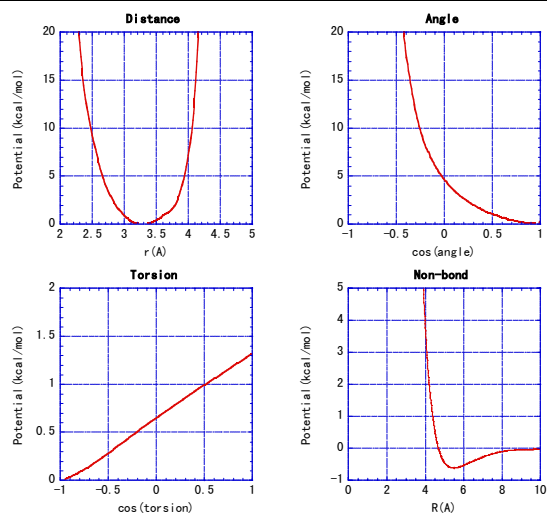


Fig.1 Coarse-grained potentials based on the distribution functions obtained by atomistic MD simulation.

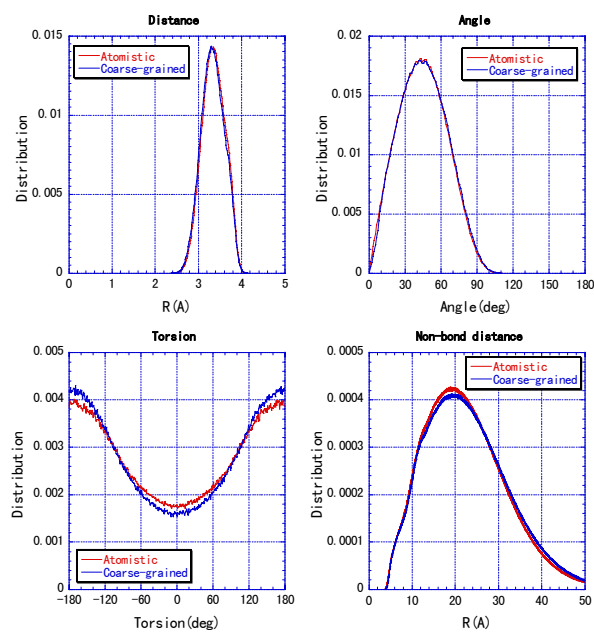


Fig.2 Comparison of distribution functions obtained by atomistic and coarse-grained MD simulations.