

run IMDElastic.pipeline - Mozilla Firefox

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IMDElastic.pipeline version 4

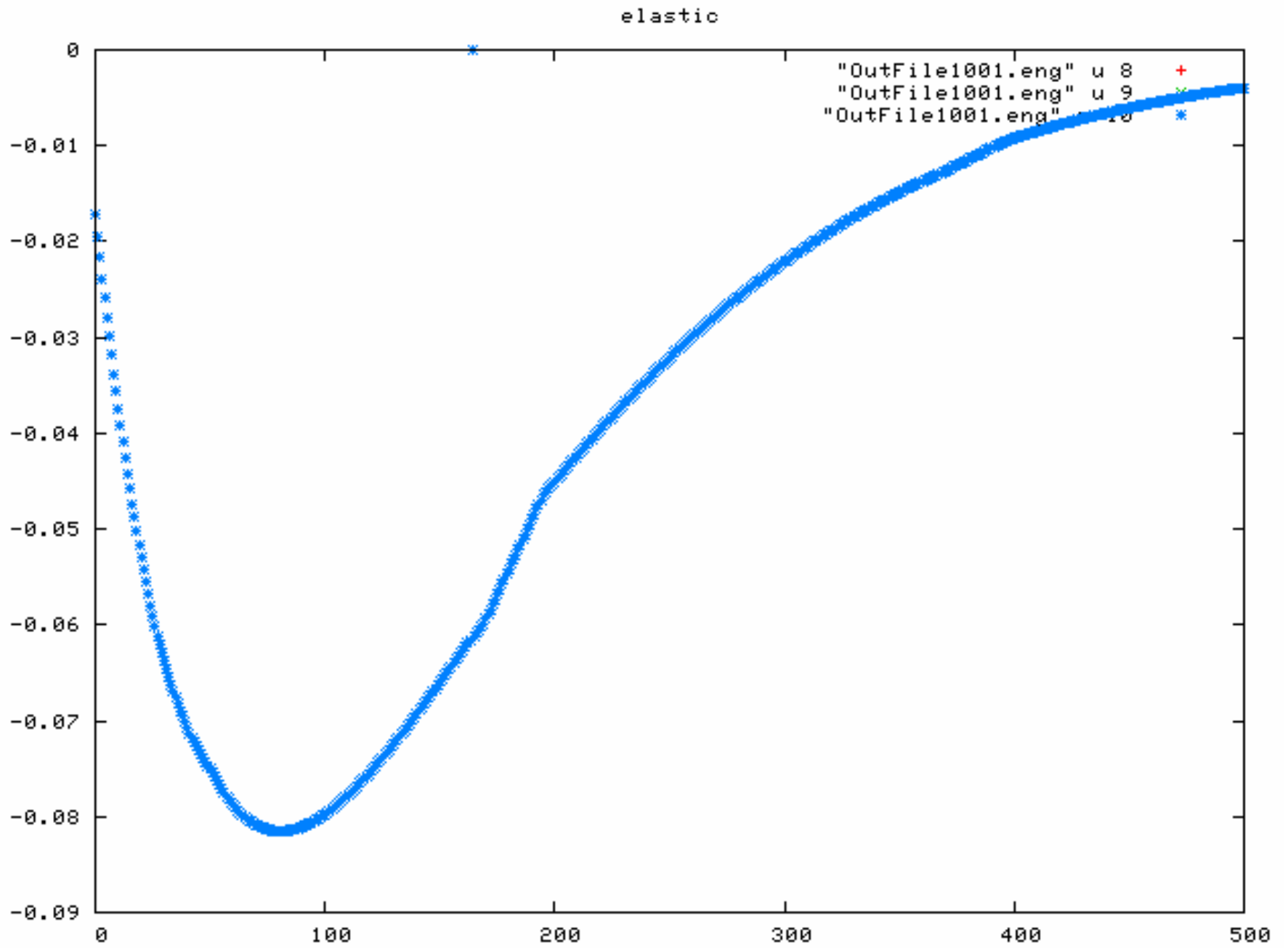
MakeCrystal1 x: *	<input type="text" value="8"/>	Dimension_x (even integer > 0)
MakeCrystal1 y: *	<input type="text" value="8"/>	Dimension_y (even integer > 0)
MakeCrystal1 z: *	<input type="text" value="8"/>	Dimension_z (even integer > 0)
IMDGetElastic2 r_cut: *	<input type="text" value="5.38"/>	Cutoff of potential
IMDGetElastic2 lj_epsilon: *	<input type="text" value=".167"/>	Lennard-Jones epsilon parameter
IMDGetElastic2 lj_sigma: *	<input type="text" value="2.314"/>	Lennard-Jones sigma parameter
IMDGetElastic2 lindef_inter: *	<input type="text" value="2"/>	Nr of steps after which is linear deformation matrix applied
IMDGetElastic2 lindef_xx: *	<input type="text" value="0.001"/>	Strain increments X
IMDGetElastic2 lindef_yy: *	<input type="text" value="0.001"/>	Strain increments Y
IMDGetElastic2 lindef_zz: *	<input type="text" value="0.001"/>	Strain increments Z
IMDGetCommon3 maxsteps: *	<input type="text" value="1000"/>	maximum # of steps
IMDGetCommon3 timestep: *	<input type="text" value="0.0001"/>	timestep (in 1.018E-014 sec)
IMDGetCommon3 pbc_x: *	<input type="text" value="1"/>	periodic BCs in X
IMDGetCommon3 pbc_y: *	<input type="text" value="1"/>	periodic BCs in Y
IMDGetCommon3 pbc_z: *	<input type="text" value="1"/>	periodic BCs in Z
IMDGetCommon3 eng_int: *	<input type="text" value="5"/>	How often is energy & stress information written
IMDGetCommon3 chkpt_int: *	<input type="text" value="2"/>	How often is chkpt information written
IMDGetCommon3 startingtemp: *	<input type="text" value="0.00000000000001"/>	Starting temperature
IMDAnimation5 energyCutoff: *	<input type="text" value="-10"/>	Energy Cut-off
IMDAnimation6 energyCutoff: *	<input type="text" value="-10"/>	Energy Cut-off
IMDAnimation7 energyCutoff: *	<input type="text" value="-10"/>	Energy Cut-off

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IMDElastic task run edit

Tr_Elastic1_prop P
stdout.txt P
Tr_Elastic.prop P
stdout.txt P
cmd.sh P
OutFile1001.eng P
imd_err.txt P
Checkpoints.zip P
EngPlot.png P
imd_out.txt P
out.xyz P
myError.log P
stdout.txt P
stderr.txt P
OutFile1001.00004.chkpt.png P
OutFile1001.00001.chkpt.png P
OutFile1001.00003.chkpt.png P
OutFile1001.00002.chkpt.png P
OutFile1001.00006.chkpt.png P
OutFile1001.00007.chkpt.png P
OutFile1001.00005.chkpt.png P
OutFile1001.00009.chkpt.png P
imd_out.txt P
OutFile1001.00010.chkpt.png P
OutFile1001.00008.chkpt.png P

IMDElastic.pipeline version 4

MakeCrystal1 x: * Dimension_x (even integer > 0)

MakeCrystal1 y: * Dimension_y (even integer > 0)

MakeCrystal1 z: * Dimension_z (even integer > 0)

IMDGetElastic2 r_cut: * Cutoff of potential

IMDGetElastic2 lj_epsilon: * Lennard-Jones epsilon parameter

IMDGetElastic2 lj_sigma: * Lennard-Jones sigma parameter

IMDGetElastic2 lindef_inter: * Nr of steps after which is linear deformation matrix applied

IMDGetElastic2 lindef_xx: * Strain increments X

IMDGetElastic2 lindef_yy: * Strain increments Y

IMDGetElastic2 lindef_zz: * Strain increments Z

IMDGetCommon3 maxsteps: * maximum # of steps

IMDGetCommon3 timestep: * timestep (in 1.018E-014 sec)

IMDGetCommon3 pbc_x: * periodic BCs in X

IMDGetCommon3 pbc_y: * periodic BCs in Y

IMDGetCommon3 pbc_z: * periodic BCs in Z

IMDGetCommon3 eng_int: * How often is energy & stress information written

IMDGetCommon3 chkpt_int: * How often is chkpt information written

IMDGetCommon3 startingtemp: * Starting temperature

IMDAnimation5 energyCutoff: * Energy Cut-off

IMDAnimation6 energyCutoff: * Energy Cut-off

IMDAnimation7 energyCutoff: * Energy Cut-off

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