

# ***Supplementary Material for KUSP: Python server for deploying ML interatomic potentials***

Amit Gupta\* and Ellad B. Tadmor†  
*Aerospace Engineering and Mechanics, University of Minnesota*

Stefano Martiniani‡  
*Center for Soft Matter Research, Department of Physics, New York University, New York 10003, USA*  
*Simons Center for Computational Physical Chemistry, Department*  
*of Chemistry, New York University, New York 10003, USA and*  
*Courant Institute of Mathematical Sciences, New York University, New York 10003, USA*

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\* gupta839@umn.edu

† tadmor@umn.edu; Equal contribution.

‡ stefano.martiniani@nyu.edu; Equal contribution.

Field	Description	Required
<code>int_width</code>	Size of integer on the system	✓
<code>n_atoms</code>	Number of atoms	
<code>atomic_numbers</code>	Atomic numbers of atoms	✓
<code>positions</code>	Positions of atoms	✓
<code>contributing_atoms</code>	Atoms to compute energy for	x

TABLE I. KUSP input data fields. These data items are received by the server from the client.

Field	Description	Required
<code>energy</code>	Energy of the system	✓
<code>forces</code>	Forces on the atoms	✓
<code>virial</code>	Virial tensor	x

TABLE II. KUSP output data fields. These data items are sent by the server to the client.

## I. KUSP INPUT AND OUTPUT DATA