ELATE: Elastic tensor analysis

Welcome to ELATE, the online tool for analysis of elastic tensors, developed by **Romain Gaillac** and **François-Xavier Coudert** at CNRS / Chimie ParisTech.
If you use the software in published results (paper, conference, etc.), please cite the corresponding paper (*J. Phys. Condens. Matter*, 2016, 28, 275201) and give the website URL.

ELATE is open source software. Any queries or comments are welcome at fx.coudert@chimie-paristech.fr

Summary of the properties (3D material)

Input: stiffness matrix (coefficients in GPa) of

```
 626.97   271.49   229.42  -0.0008  -1.4775  -0.0012
 271.49   626.97   229.42   0.0009   1.4773  -0.0005
 229.42   229.42   798.98  -0.0002   0.0009  -0.0002
-0.0008   0.0009  -0.0002   168.77  -0.0005    1.477
-1.4775   1.4773   0.0009  -0.0005   168.77  -0.0001
-0.0012  -0.0005  -0.0002    1.477  -0.0001   177.73
```

Average properties

Averaging scheme	Bulk modulus	Young's modulus	Shear modulus	Poisson's ratio
Voigt	K_V = 390.4 GPa	E_V = 493.16 GPa	G_V = 191.23 GPa	ν_V = 0.28946
Reuss	K_R = 388.02 GPa	E_R = 480.4 GPa	G_R = 185.67 GPa	ν_R = 0.29365
Hill	K_H = 389.21 GPa	E_H = 486.79 GPa	G_H = 188.45 GPa	ν_H = 0.29155

Eigenvalues of the stiffness matrix

λ_1	λ_2	λ_3	λ_4	λ_5	λ_6
168.53 GPa	168.74 GPa	177.97 GPa	355.5 GPa	520.48 GPa	1177 GPa

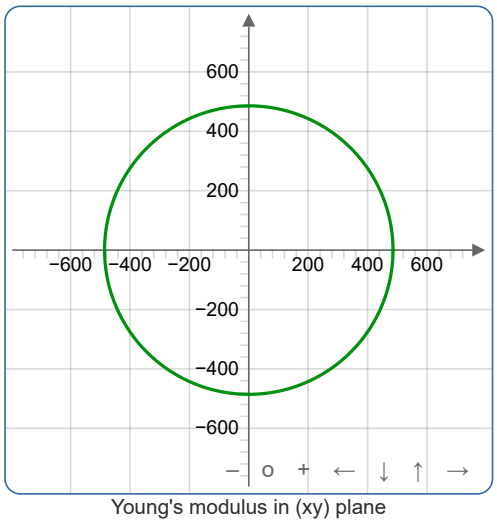
Variations of the elastic moduli

	Young's modulus		Linear compressibility		Shear modulus		Poisson's ratio		
	E_{min}	E_{max}	β_{min}	β_{max}	G_{min}	G_{max}	ν_{min}	ν_{max}	
Value	445.57 GPa	681.82 GPa	0.71764 TPa^{-1}	0.92978 TPa^{-1}	168.53 GPa	233.97 GPa	0.18171	0.37	Value
Anisotropy	1.53		1.2956		1.388		2.0362		Anisotropy
Axis	0.4132 0.7152 -0.5637	0.0000 -0.0000 1.0000	0.0000 -0.0000 1.0000	0.5309 0.8474 -0.0000	-0.1585 0.0000 0.9874	-0.7018 0.0056 0.7124	0.8642 0.5032 0.0001	-0.6235 -0.0000 0.7818	Axis

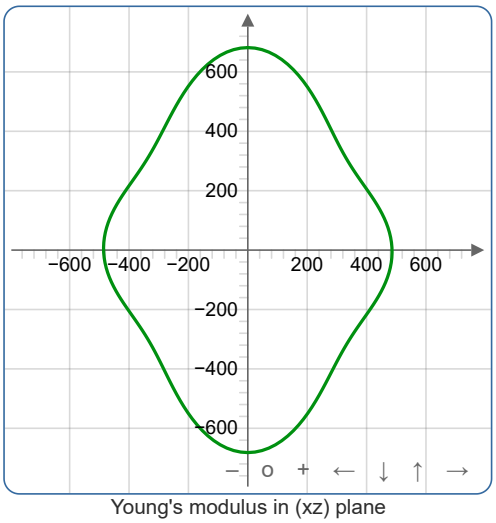
0.0002	-0.7123	0.0162	-0.7818	Second axis
1.0000	0.0054	-0.0280	-0.0001	
0.0000	-0.7018	0.9995	-0.6235	

Spatial dependence of Young's modulus

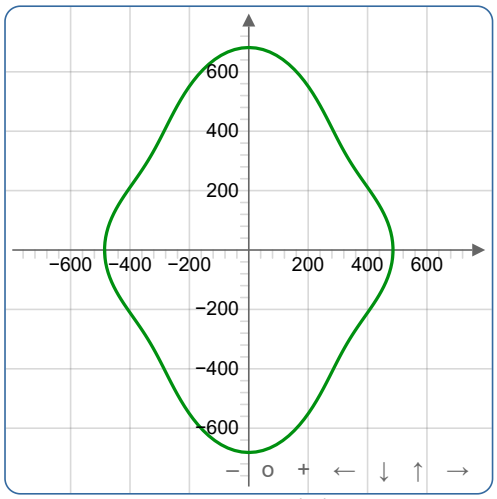
Visualize in 3D



Young's modulus in (xy) plane



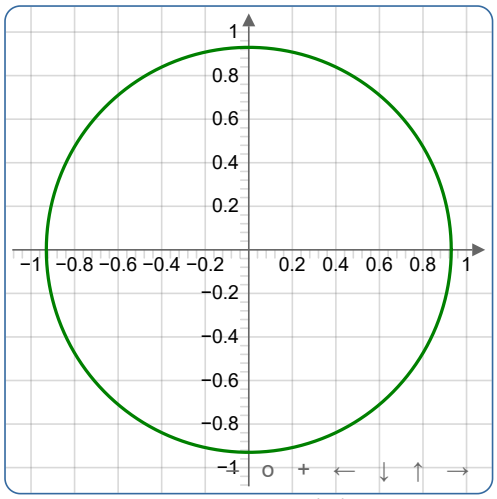
Young's modulus in (xz) plane



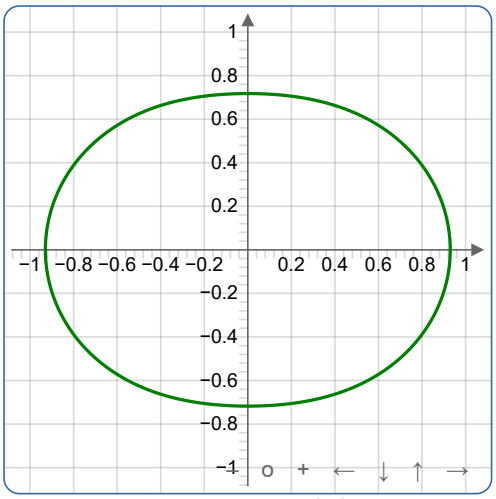
Young's modulus in (yz) plane

Spatial dependence of linear compressibility

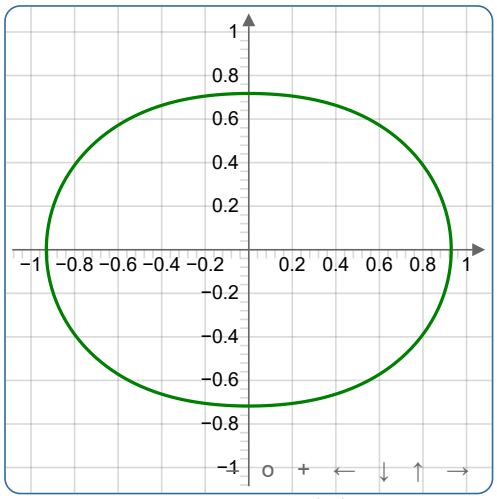
Visualize in 3D



linear compressibility in (xy) plane



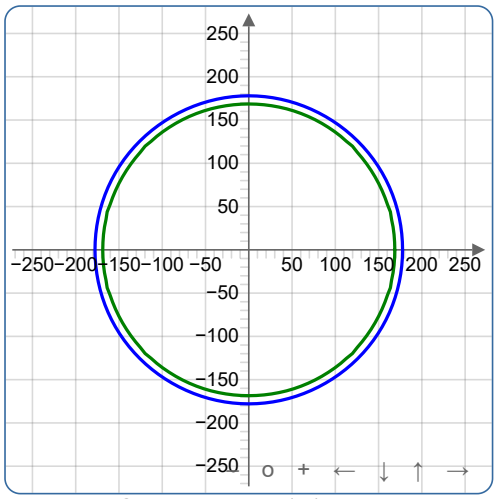
linear compressibility in (xz) plane



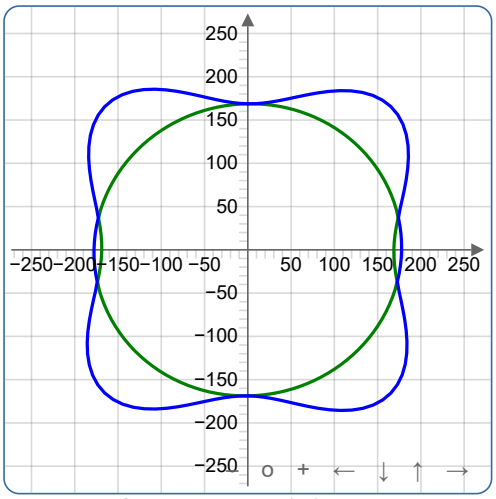
linear compressibility in (yz) plane

Spatial dependence of shear modulus

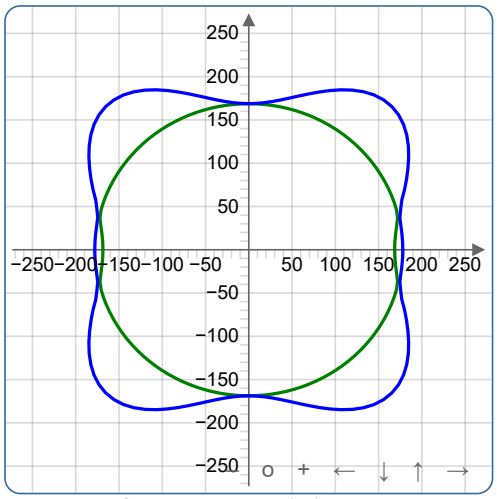
Visualize in 3D



Shear modulus in (xy) plane



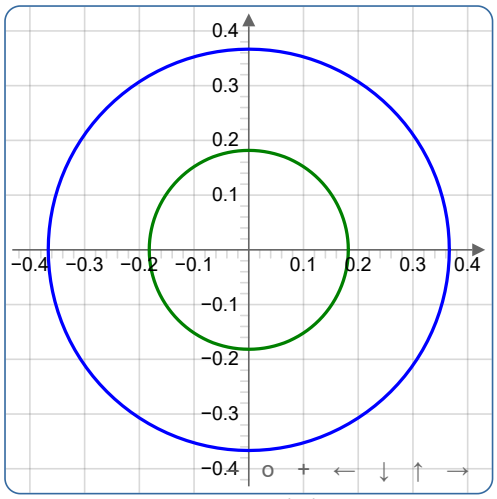
Shear modulus in (xz) plane



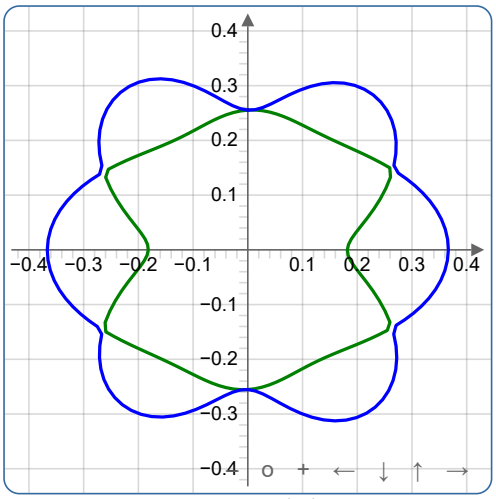
Shear modulus in (yz) plane

Spatial dependence of Poisson's ratio

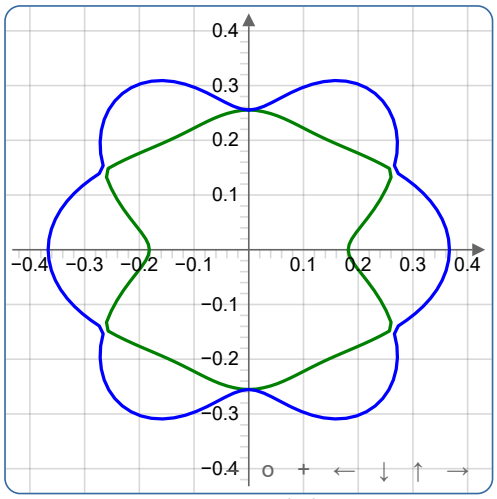
Visualize in 3D



Poisson's ratio in (xy) plane



Poisson's ratio in (xz) plane



Poisson's ratio in (yz) plane

Code version: 2024.03.15 (running on Python 3.11.2)
Execution time: 0.896 seconds