

MESHI* – a new object oriented package for molecular simulations

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* **Meshi** – the Hebrew name of the splendid protein **silk**.

(and a tribute to CK's late cat)

Thanks to:

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- My group members in BGU: Nir Kalisman, Ami Levi, Sharon Zafri-lynn, Tetyana Maxymova and Yan Gleyzer.
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- The four masters : R. Elber, J. Skolnik, A. Kolinski and M. Levitt.

Why a new package

new
idea

Fortran/C programs dominate the field of computational structural biology. Some of them are master pieces.

- 😊 Fortran/C compilers are very well optimized.
- 😊 A huge corpus of reliable code already exists.
- 😞 Fortran/C programs are inherently hard to comprehend and not as modular as we tend to think.
- 😞 These programs tends to be oriented towards computational efficiency.

implementation



new
idea

We believe that the most precious
resource is developer's time.
Moore's law does not apply to it

implementation

Why Java

- ☹️ **Java is around two times slower than C++.**
- ☹️ **You always need to defend its usage.**
- 😊 **There are quite a few bugs you cannot do in Java.**
- 😊 **Java forces you to write in an object oriented fashion.**
- 😊 **One can always write the (few) computational bottlenecks in Fortran/C/assembly language.**

The modular, object oriented
approach of MESHI.

Sample classes

Coordinates

Coordinates

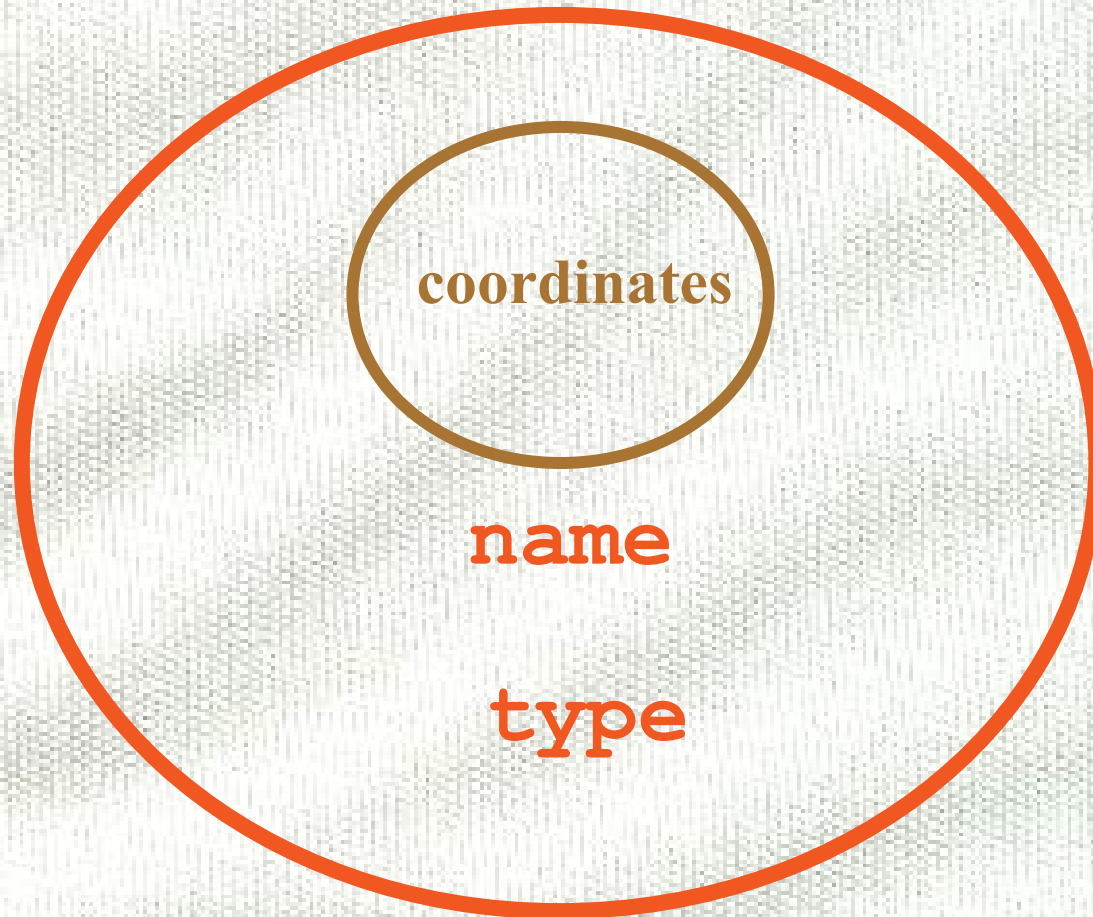
X Y Z

Forces

F_X F_Y F_Z



Atom



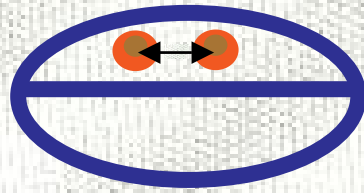
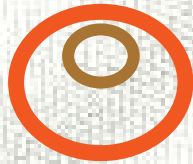


Distance

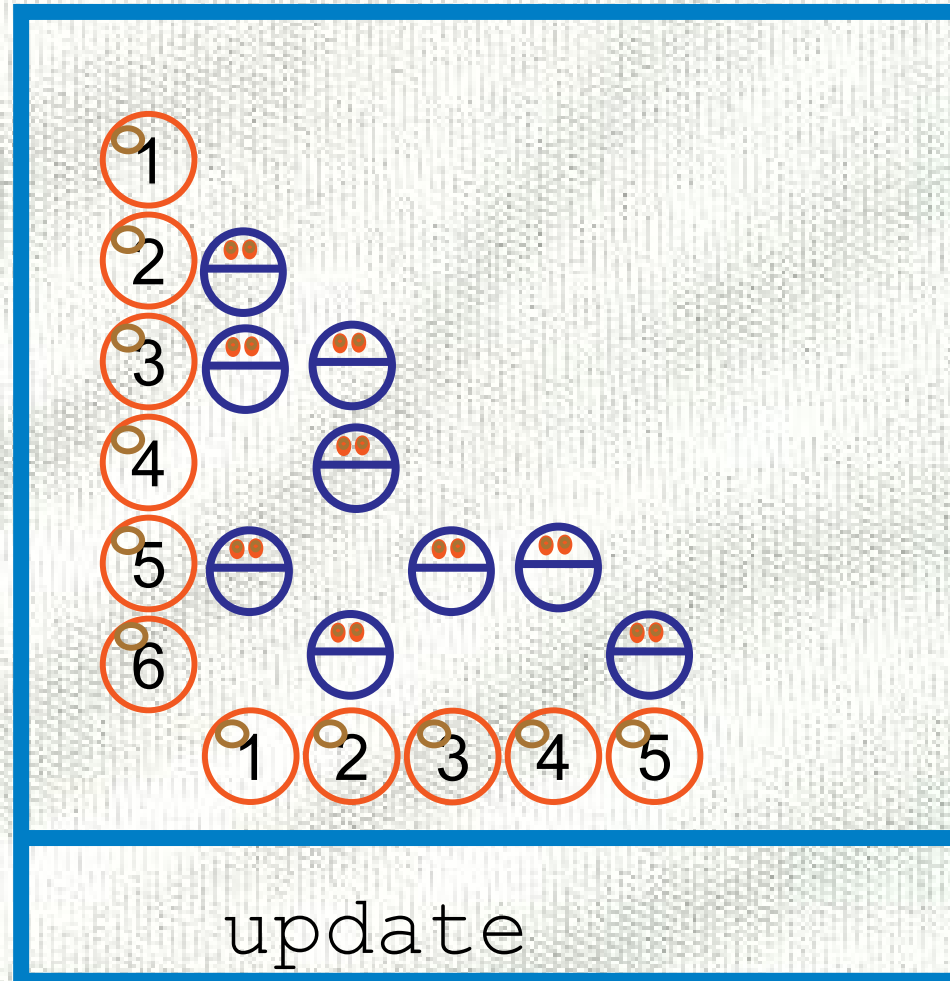
atom1 atom2

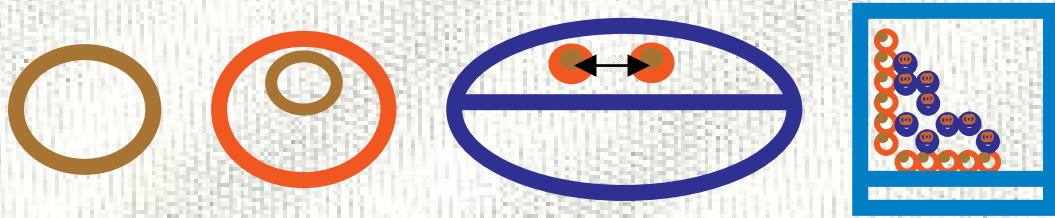
$\frac{1}{d}$ d d^2 $\frac{\partial d}{\partial X}$ $\frac{\partial d}{\partial Y}$ $\frac{\partial d}{\partial Z}$

update

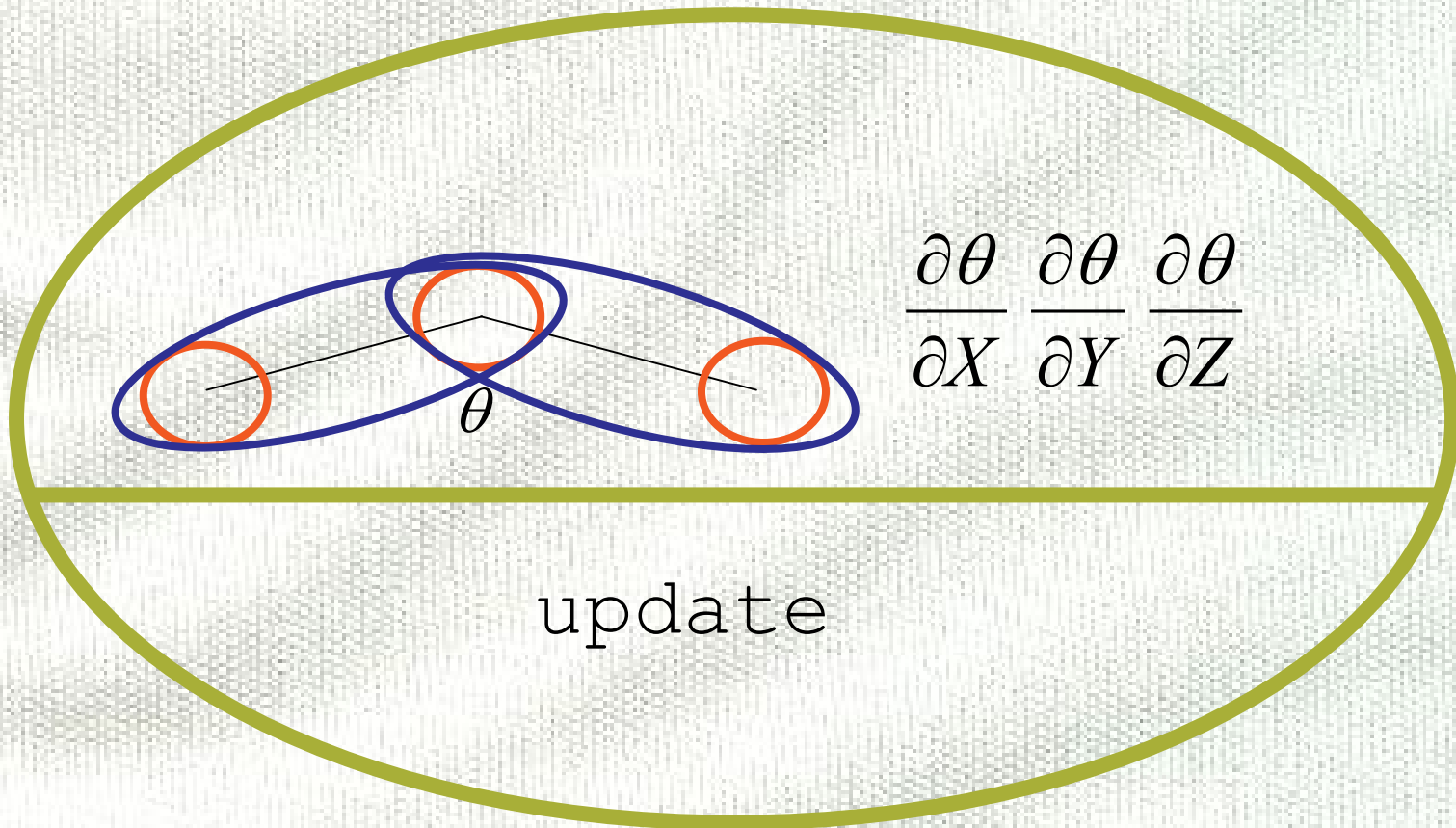


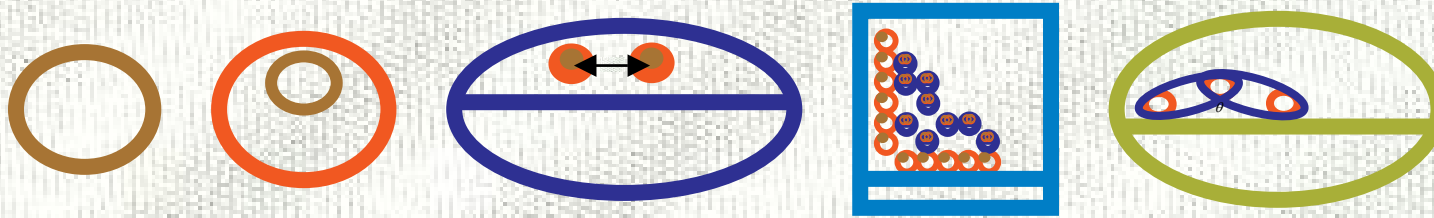
DistanceMatrix





Angle





AngleEnergyElement

Atom type specific
constants



$\bar{\theta}$

K

1. Evaluate $e_{\theta} = K(\theta - \bar{\theta})^2$

2. Update **atom** forces

AngleEnergyElement (sub-class of EnergyElement)

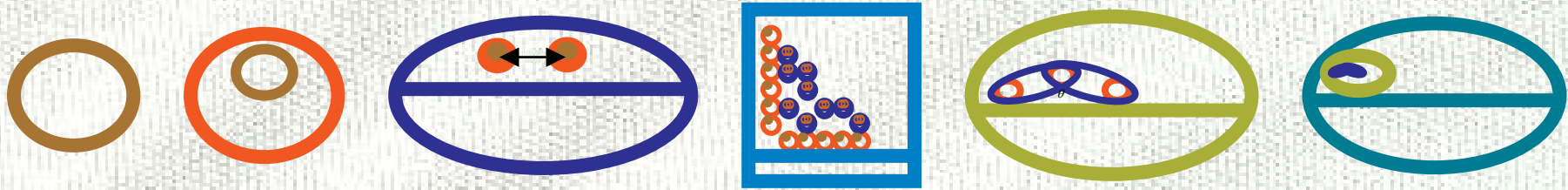
Atom type specific
constants



$\bar{\theta}$

K

3.Test (inherited form
EnergyElement).



AngleEnergy

A list of elements



1. Evaluate $E_{angle} = \sum_{\theta} e_{\theta}$
2. Update **atom** forces



TotalEnergy

1. Update `DistanceMatrix`
2. Evaluate $E_{total} = \sum_{term} e_{term}$
3. Update `atom` forces



LBFGS

(minimizer)

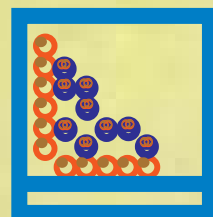
A list of coordinates



1. Update energy and forces
2. Change the coordinates according to the forces.
3. If not yet in a minimum - go to 1.

Current Meshi projects

- ✱ Novel algorithm for non-bonded-list generation.

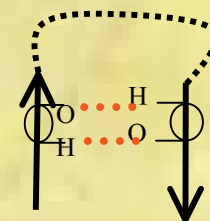


- ✱ MCMM-like stochastic optimization.

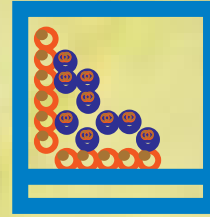


- ✱ Continues knowledge-based potential for pairs of torsion angles.

- ✱ Cooperative hydrogen-bonds potential.



generation.

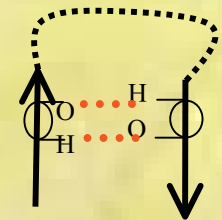


✱ MCMM-like stochastic optimization.



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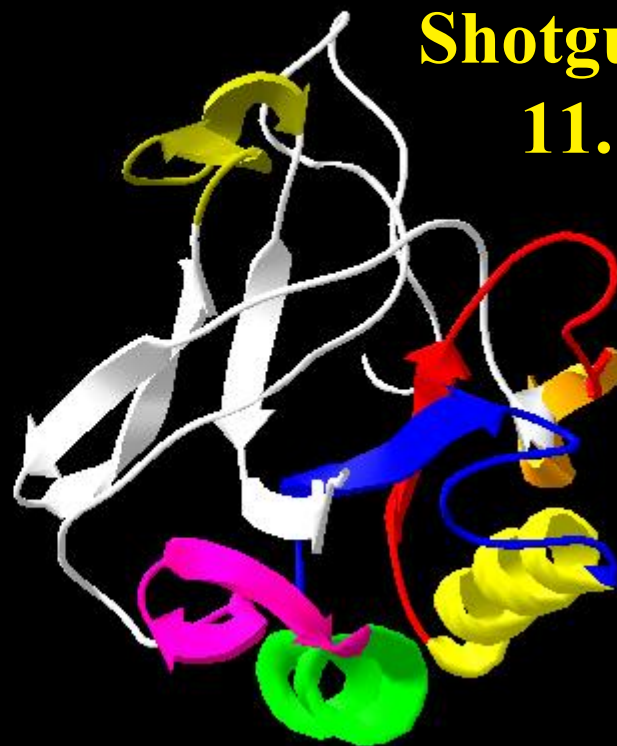
✱ Cooperative hydrogen-bonds potential.



✱ A refinement program for fold-recognition models.

Shotgun
12.5Å (7.4)

1NXJ – T0156



www.cs.bgu.ac.il/~meshi

Documentation and results are not as good as they should be, but they are (well at least the documentation) improving.