MESHI* – a new object oriented package for molecular simulations

Nir Kalisman, Ami Levi, Sharon Zafriri-lynn, Ram Janovski, Tetyana Maxymova, Yan Gleyzer, Dan Reshef and Chen Keasar

Departments of Computer Science and Life Sciences BGU

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

(and a tribute to CK's late cat)

Thanks to:

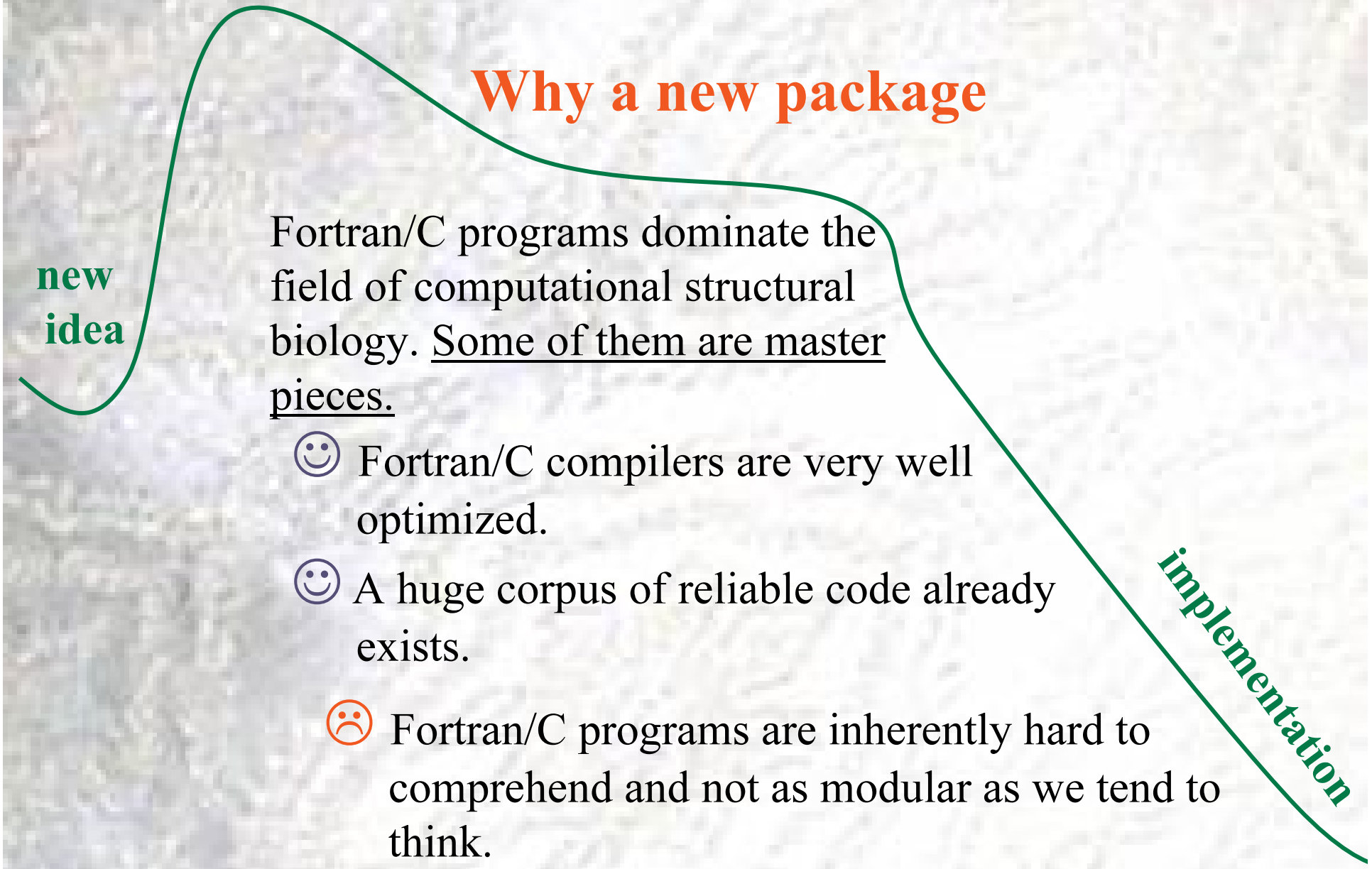
- Organizers and assessors.

- My group members in BGU: Nir Kalisman, Ami Levi, Sharon Zafriri-lynn, Tetyana Maxymova and Yan Gleyzer.

- The GeneFun consortium.

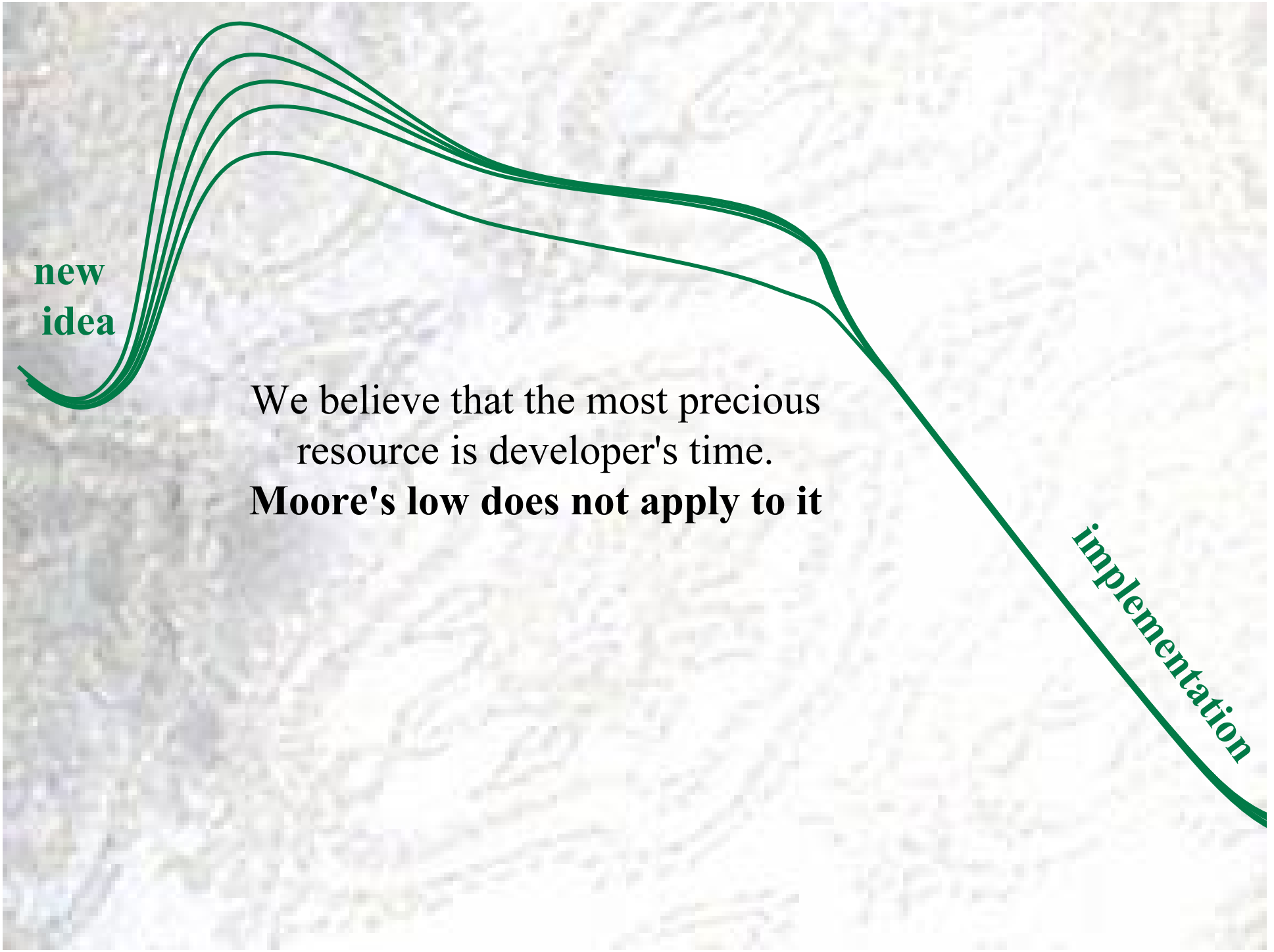
- The four masters : R. Elber, J. Skolnik, A. Kolinski and M. Levitt.

Why a new package



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.


new
idea
We believe that the most precious
resource is developer's time.
Moore's low does not apply to it
implementation

Why Java

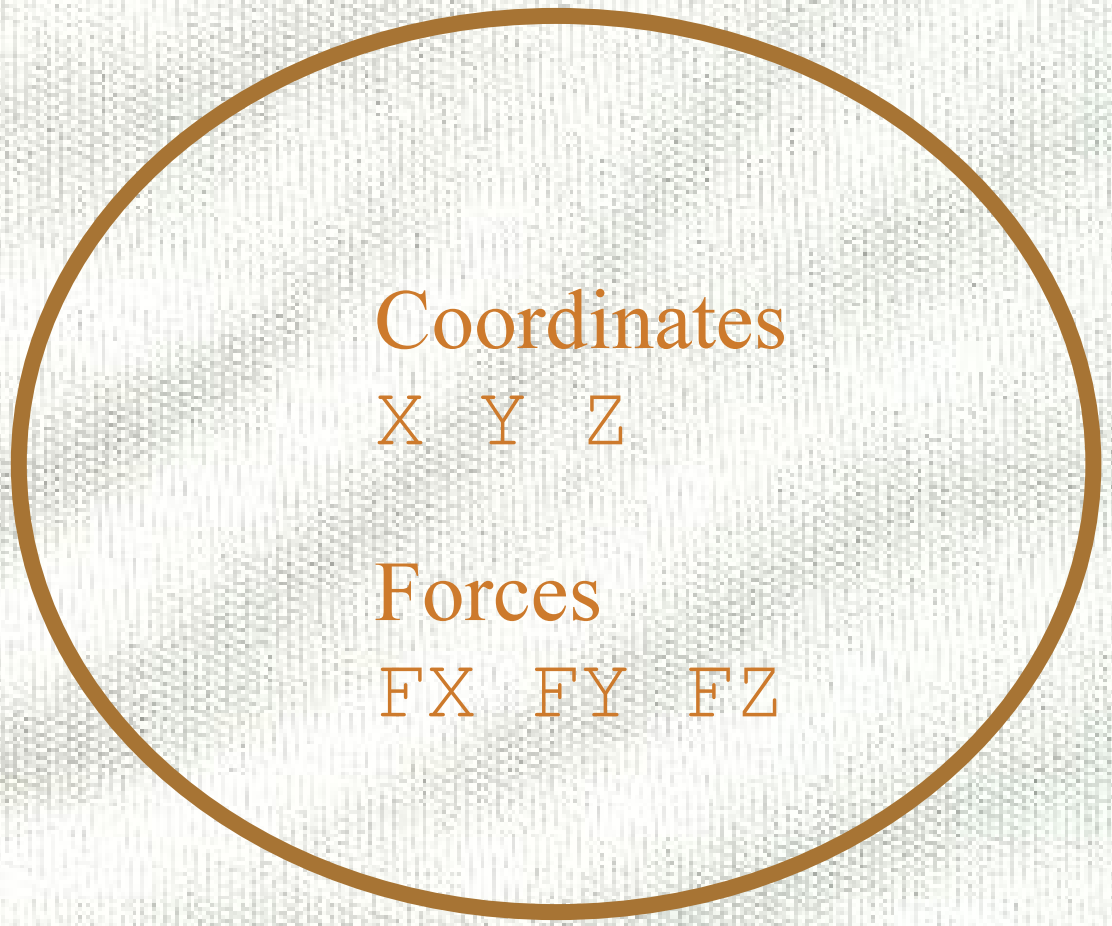
- ☹ Java is around two times slower than C++.
- ☹ You always need to defend its usage.

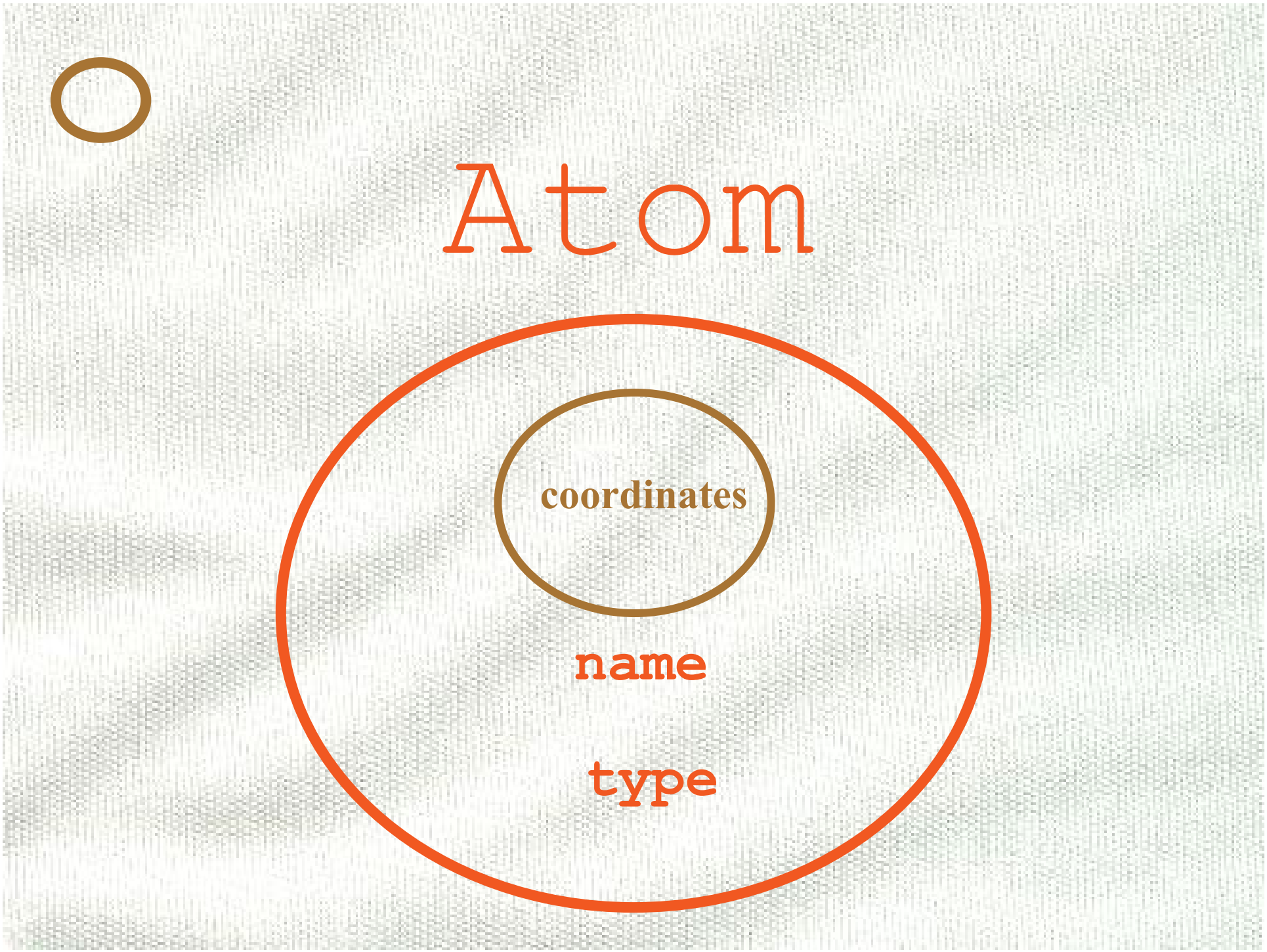
- ☺ There are quite a few bugs you cannot do in Java.
- ☺ Java forces you to write in an object oriented fashion.
- ☺ One can always write the (few) computational bottlenecks in Fortran/C/assembly language.

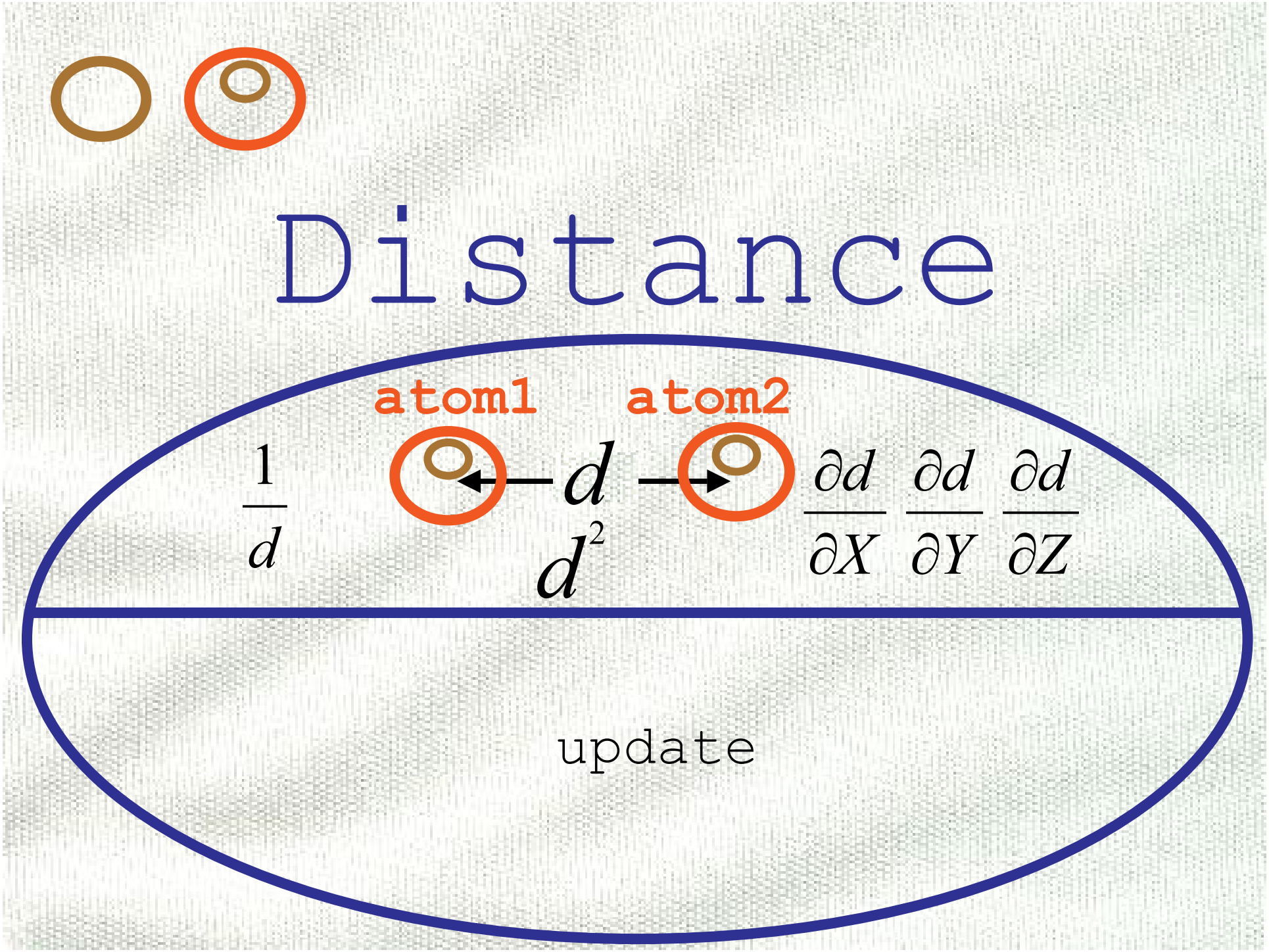
The modular, object oriented approach of MESHI.

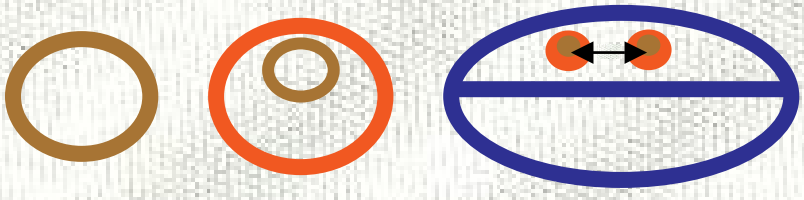
Sample classes

Coordinates

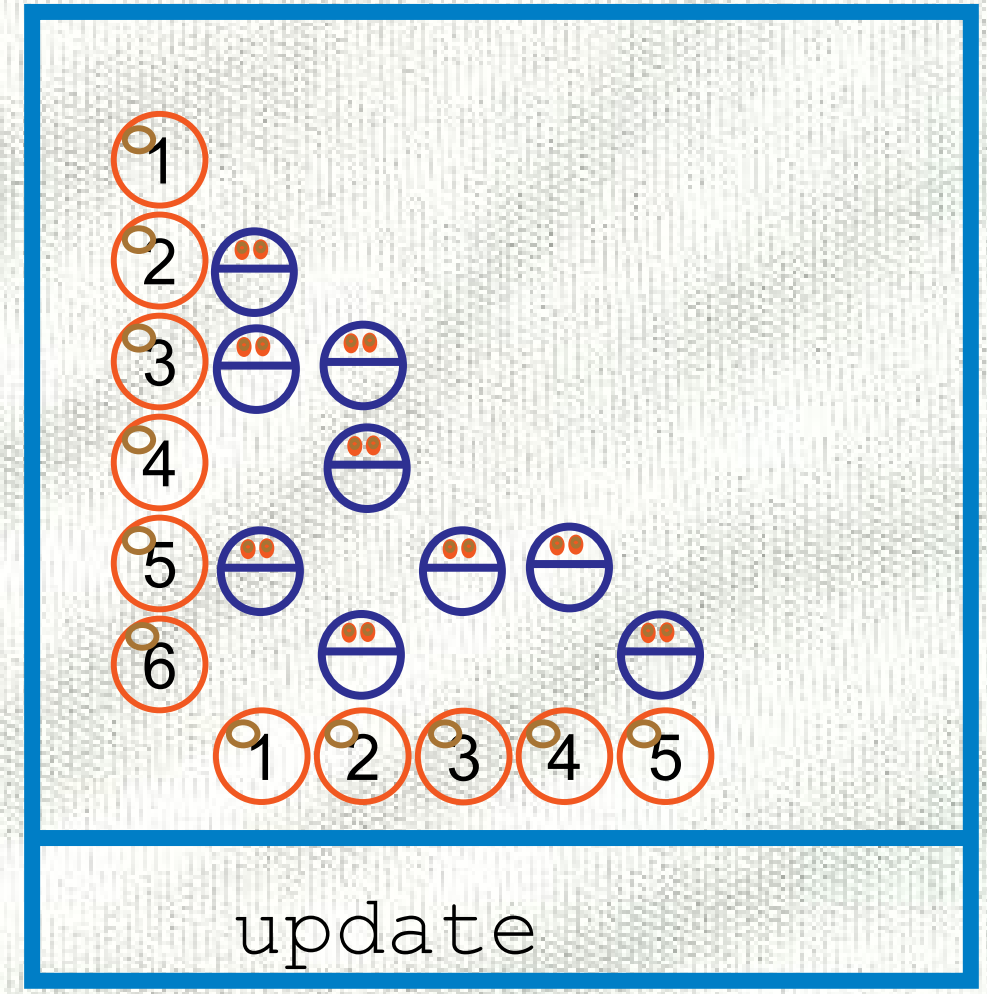


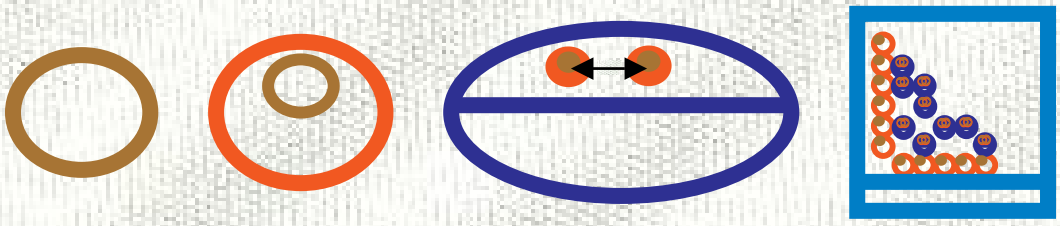

Atom
coordinates
name
type


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

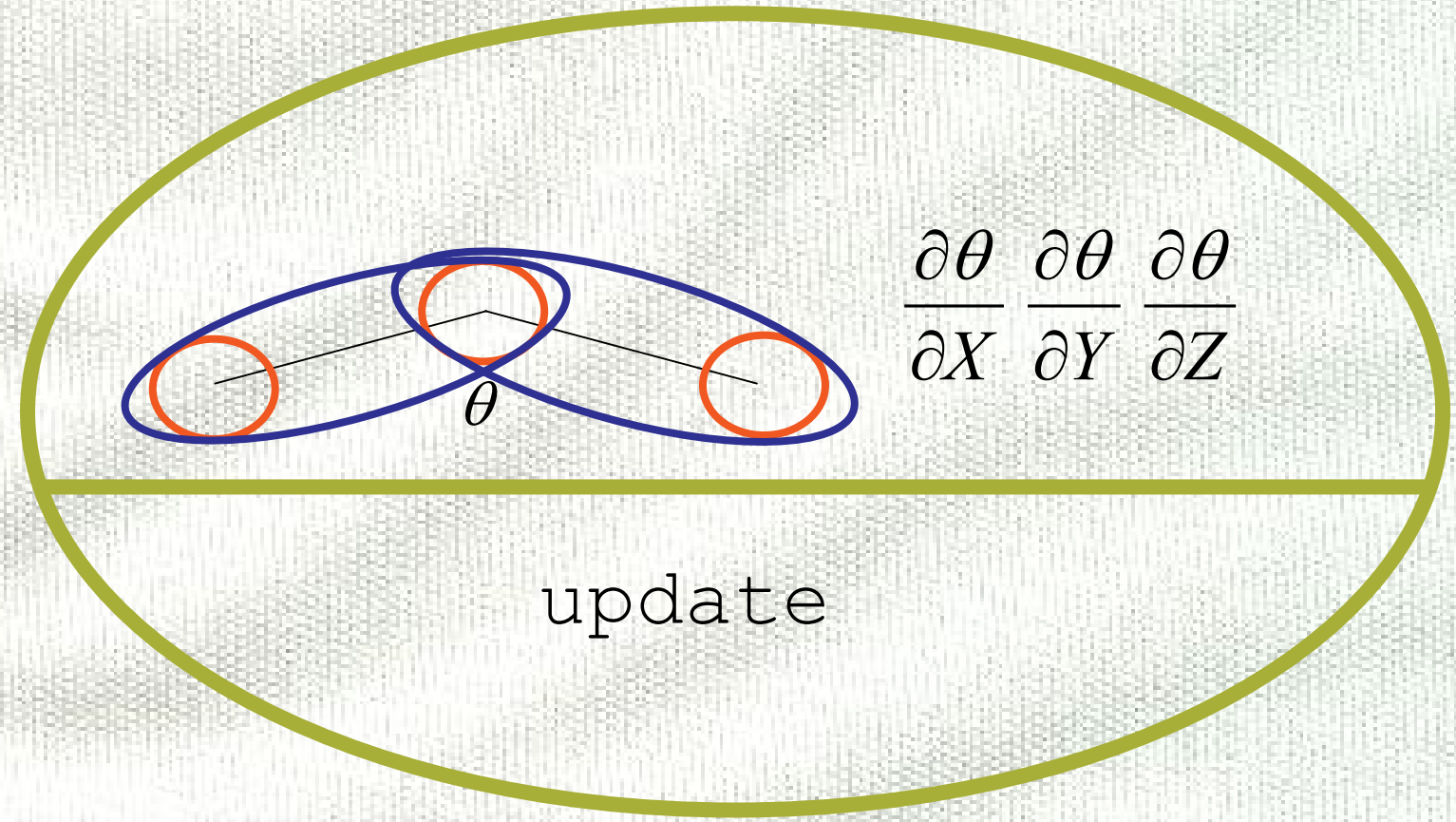


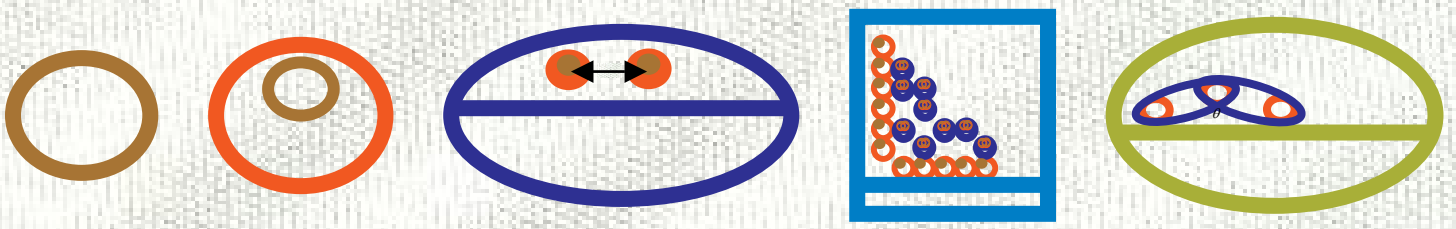
DistanceMatrix





Angle


θ
$\frac{\partial\theta}{\partial X}\ \frac{\partial\theta}{\partial Y}\ \frac{\partial\theta}{\partial Z}$
update



AngleEnergyElement

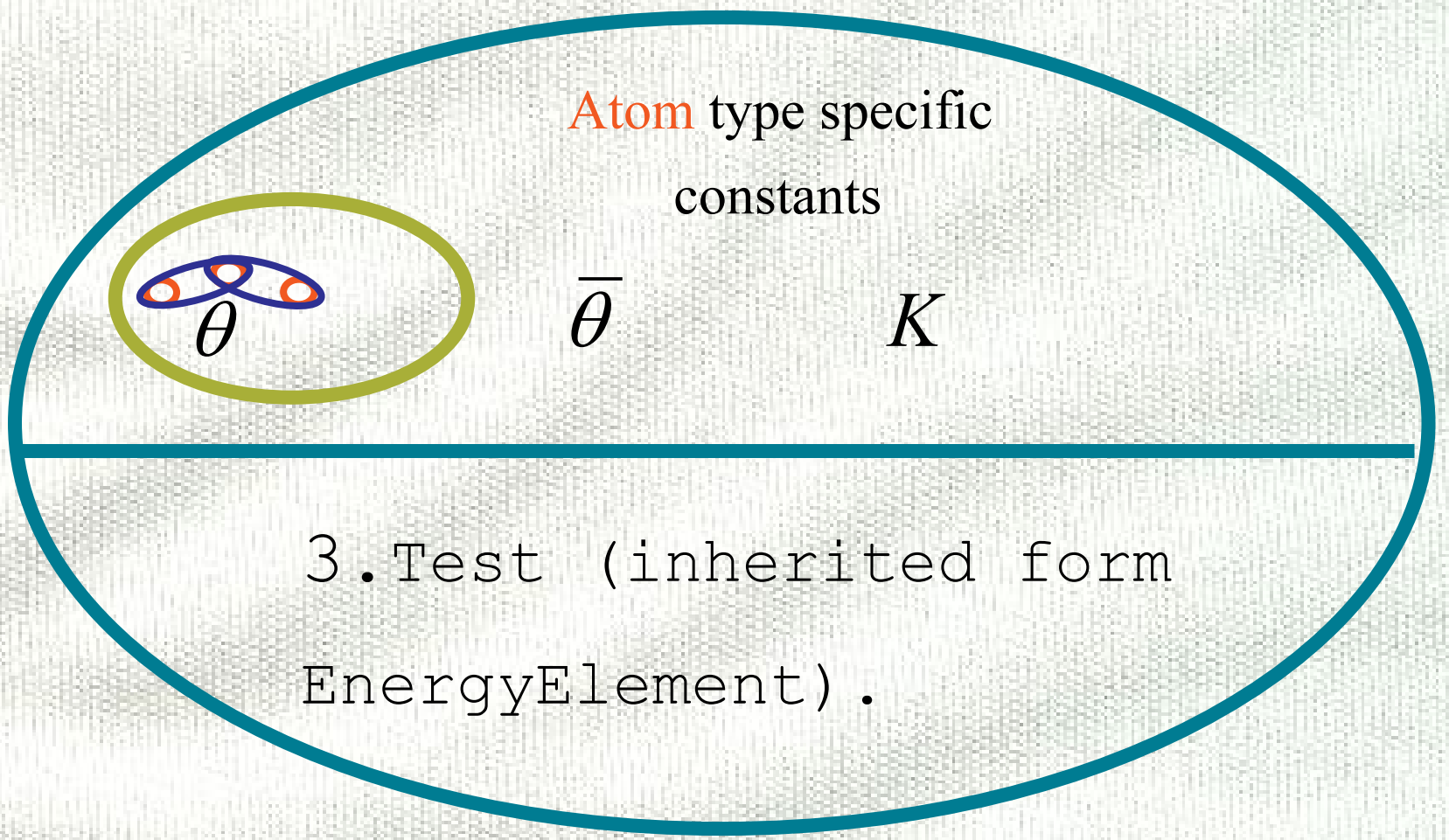
Atom type specific constants

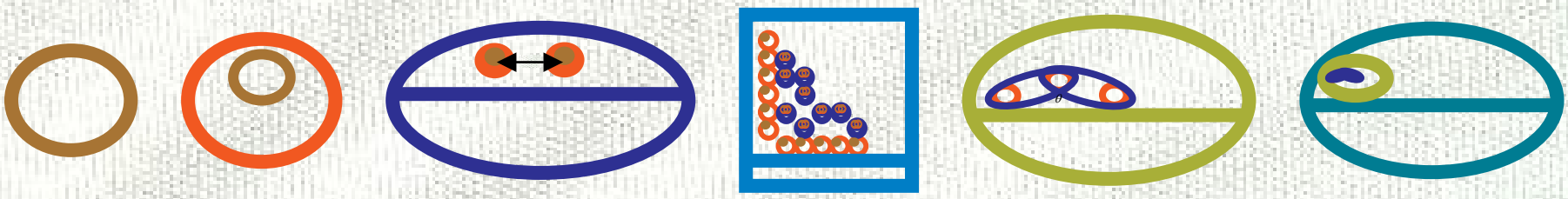
$\bar{\theta}$ K

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

2. Update **atom** forces

AngleEnergyElement (sub-class of EnergyElement)



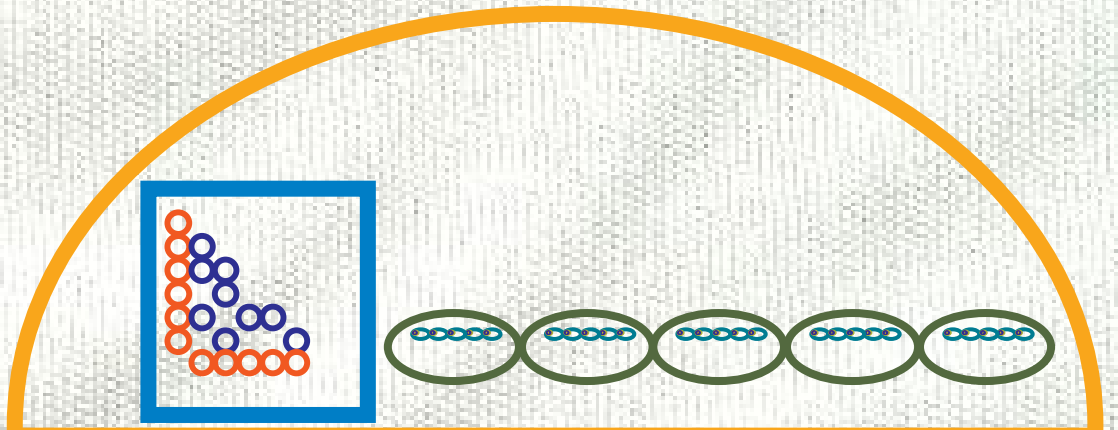


AngleEnergy

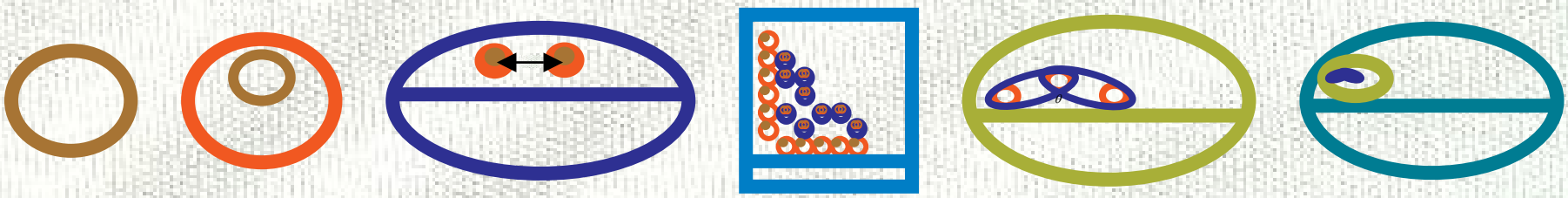
A list of elements

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

TotalEnergy

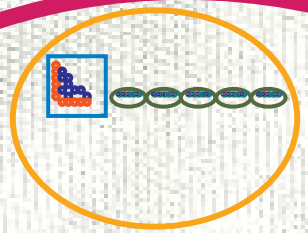


1. Update DistanceMatrix
2. Evaluate $E_{total} = \sum_{term} e_{term}$
3. Update **atom** forces



LBFGS

(minimizer)

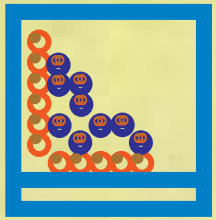


A list of coordinates

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

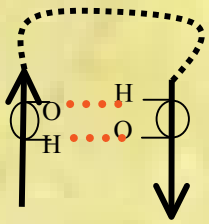
Current Meshi projects

- Novel algorithm for non-bonded-list generation.

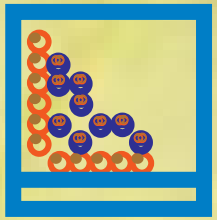


- MCMM-like stochastic optimization.

- Continues knowledge-based potential for pairs of torsion angles.
- Cooperative hydrogen-bonds potential.



generation.



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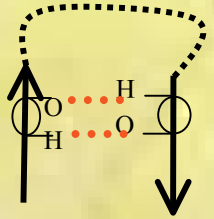
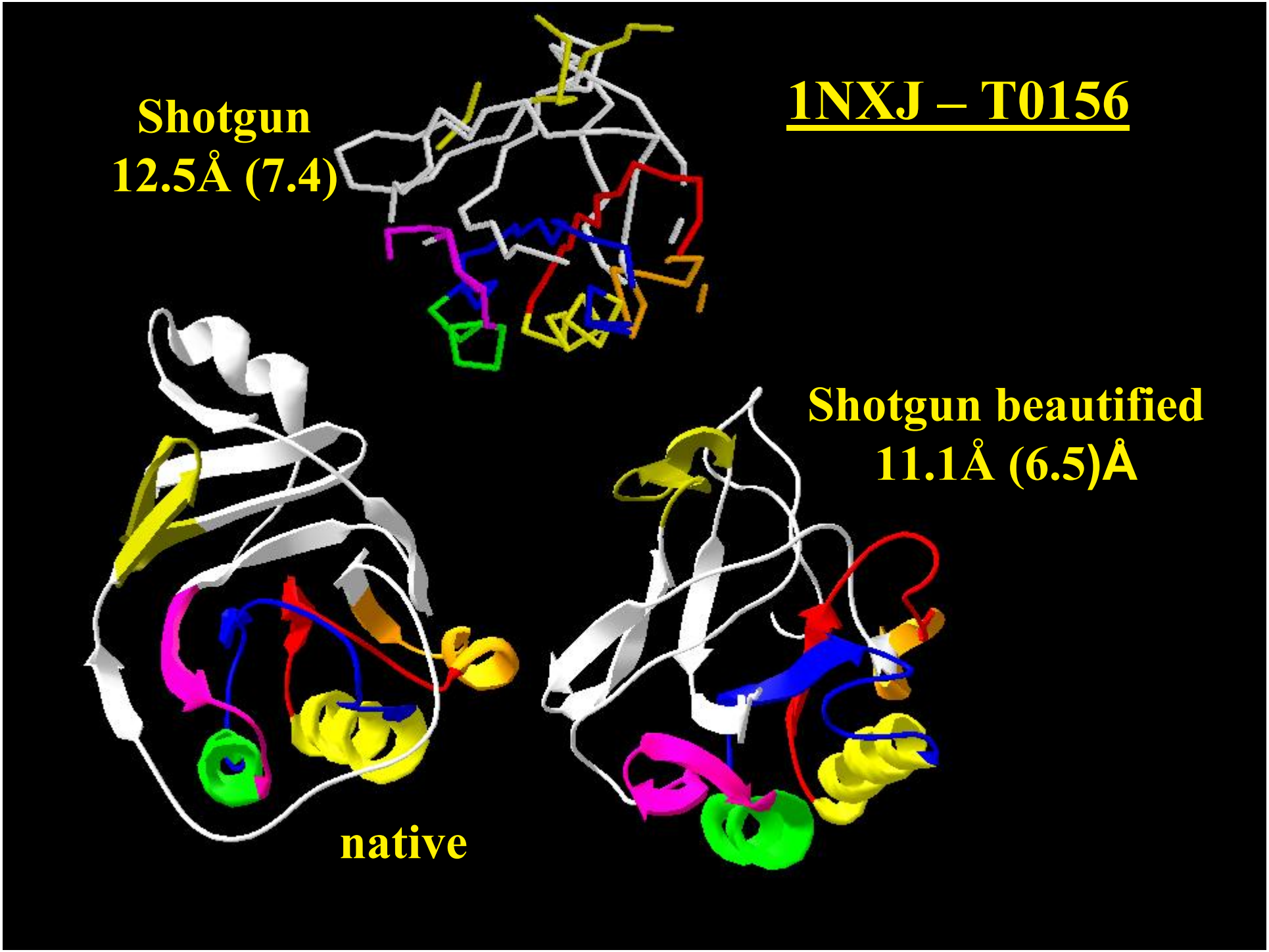


- A refinement program for fold-recognition models.


1NXJ – T0156
Shotgun
12.5Å (7.4)
Shotgun beautified
11.1Å (6.5)Å
native

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.