Ecole Thématique "Plasmonique Moléculaire et Spectroscopies Exaltées"
Cours, ateliers pratiques, visites, posters, table ronde
20-24 juin 2016 Toulouse (France)

ATELIER 2: Simulations numériques des propriétés optiques

Objectif:

Cet atelier d'une durée de 2h45 vise à présenter de façon pratique deux techniques permettant de simuler les propriétés optiques de nanostructures plasmoniques couramment utilisées aujourd'hui: l'approximation des **dipôles discrets** (*DDA, Discrete Dipole Approximation*) et la méthode des **différences finies** dans le domaine temporel (*FDTD, Finite Difference Time Domain*).

L'objectif de cet atelier n'est pas une présentation détaillée du cadre théorique de ces méthodes mais une **introduction pratique** à leur fonctionnement et leur **utilisation sur quelques exemples simples**. Le code DDSCAT développé par Bruce T. Draine et Piotr J. Flatau sera utilisé pour introduire la méthode DDA (DDSCAT 7.3). La méthode des différences finies sera elle illustrée grâce au logiciel MEEP développé au MIT.

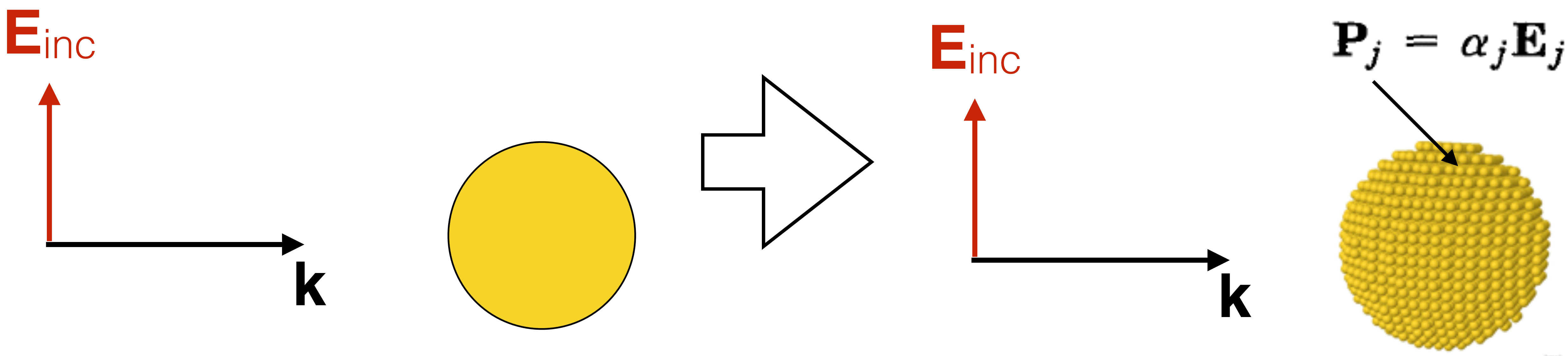
Les principes généraux de fonctionnement de ces outils, et en particulier

- la définition de la géométrie étudiée
- la définition des paramètres d'illumination
- les observables accessibles

seront présentés sur quelques exemples simples.

The Discrete Dipole Approximation

DDA replaces a **continuum target** by an array of **point dipoles** : Draine & Flatau, J. Opt. Soc. Am. A, 11, 1491, **1994**



The field at any point of the lattice is the sum of the incident field + the E-fields radiated by the other dipoles

$$\boxed{\mathbf{E}_j = \mathbf{E}_{\mathrm{inc},j} - \sum_{k \neq j} \mathbf{A}_{jk} \mathbf{P}_k}$$

$$\mathbf{A}_{jk} = \frac{\exp(ikr_{jk})}{r_{jk}} \times \left[k^2 (\hat{r}_{jk}\hat{r}_{jk} - \mathbf{1}_3) + \frac{ikr_{jk} - 1}{{r_{jk}}^2} (3\hat{r}_{jk}\hat{r}_{jk} - \mathbf{1}_3) \right] \quad j \neq k$$

$$\boxed{\sum_{k=1}^{N} \mathbf{A}_{jk} \mathbf{P}_k = \mathbf{E}_{\mathrm{inc},j}}$$

$$\mathbf{A}_{jj} \equiv {\alpha_j}^{-1}$$

Inversion problem with 3N unknowns (P_k) solved iteratively

$$r_{jk} \equiv |\mathbf{r}_j - \mathbf{r}_k| \qquad \hat{r}_{jk} \equiv (\mathbf{r}_j - \mathbf{r}_k)/r_{jk} \qquad k \equiv \omega/c$$

The Discrete Dipole Approximation

Once $\mathbf{P}_k$ is know, the optical response can be calculated.

For instance, the **extinction, absorption** and **scattering cross-sections :**

$$\boxed{C_{\text{ext}} = \frac{4\pi k}{|\mathbf{E}_0|^2} \sum_{j=1}^{N} \text{Im}(\mathbf{E}_{\text{inc},j}{}^* \cdot \mathbf{P}_j)\,,}$$

$$\boxed{C_{\text{abs}} = \frac{4\pi k}{|\mathbf{E}_0|^2} \sum_{j=1}^{N} \left\{ \text{Im}[\mathbf{P}_j \cdot (\alpha_j{}^{-1})^* \mathbf{P}_j{}^*] - \frac{2}{3} k^3 |\mathbf{P}_j|^2 \right\}}$$

$$\boxed{C_{\text{sca}} = C_{\text{ext}} - C_{\text{abs}}}$$

The parameters

All key parameters of a computation are contained in a parameter file called *ddscat.par*

This file contains all informations about :

Illumination Wavelength of incident EM wave + polarization

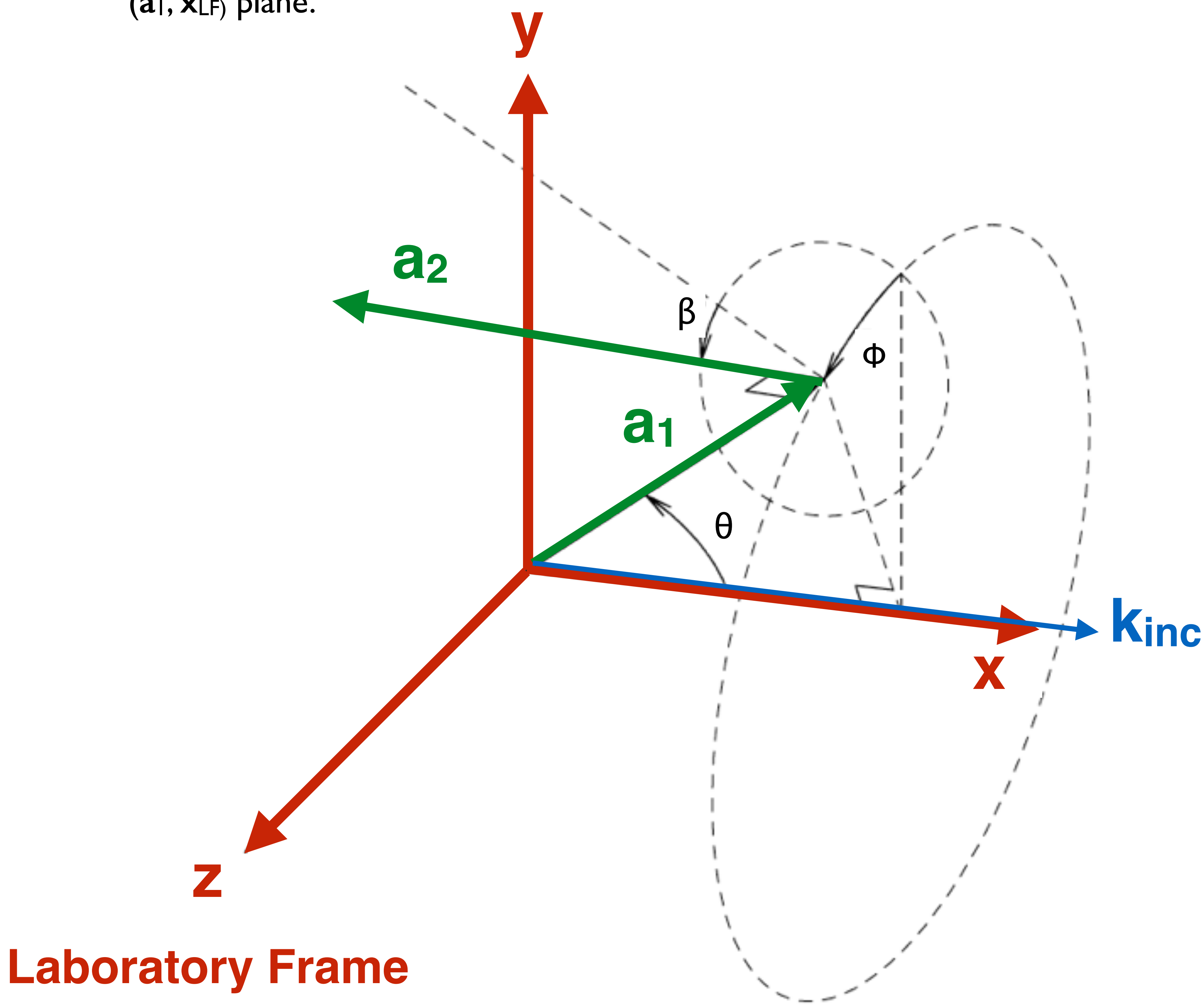
Nano-object Position of lattice points - Dielectric constants of all materials

Computation Resolution method - Output desired - accuracy required and max. iterations

Target orientation in the Lab Frame

x = **x**$_{LF}$ is the direction of propagation of the incident radiation, and **y** = **y**$_{LF}$ is the direction of the first incident polarization.

The orientation of target axis **a**$_1$ is specified by angles θ and Φ. The orientation of target axis **a**$_2$ is then determined by angle β specifying rotation of the target around **a**$_1$. **Example:** when β = 0, **a**$_2$ lies in the (**a**$_1$, **x**$_{LF}$) plane.



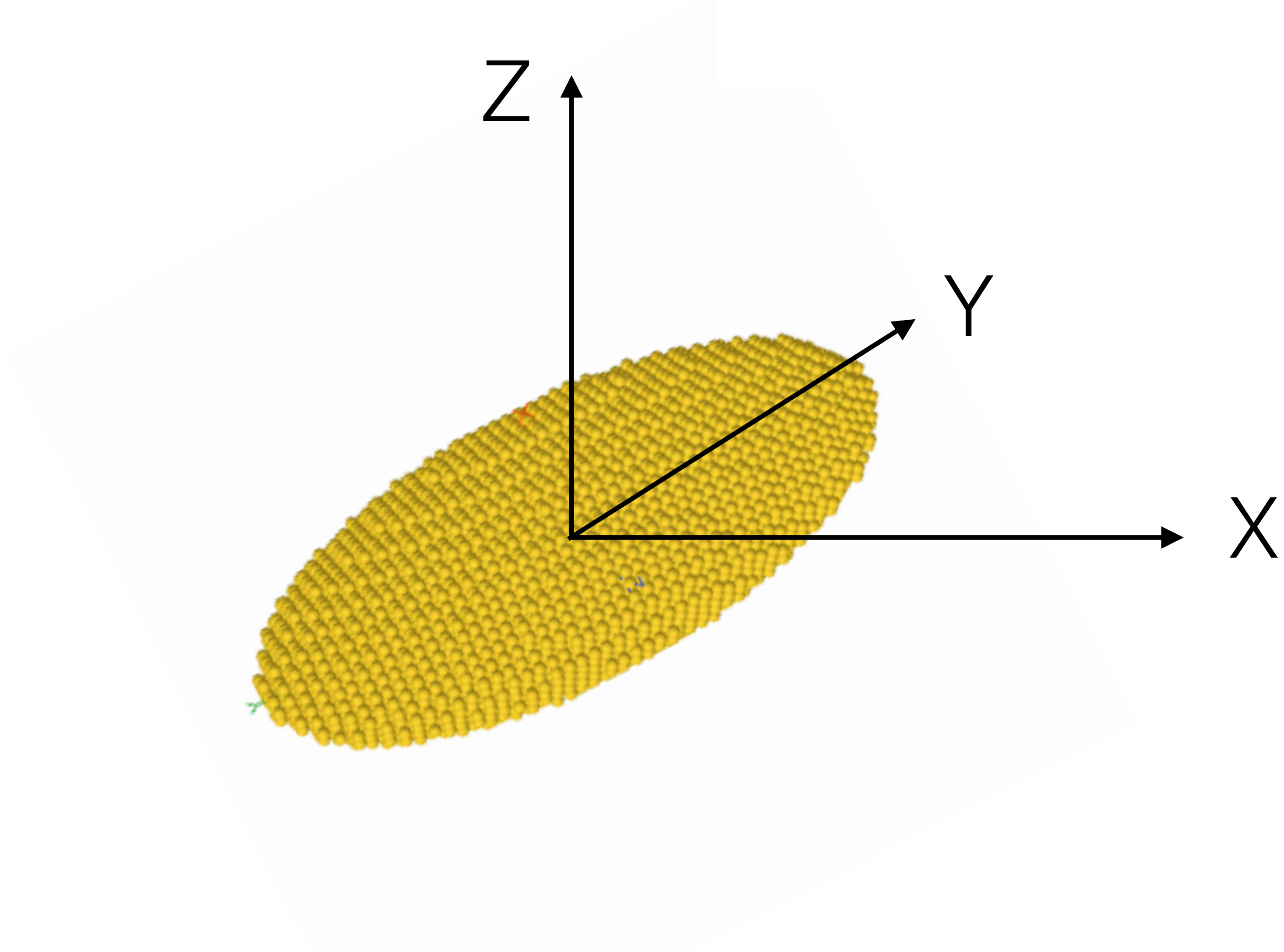
Predefined Shape : ELLIPSOID

21.12 ELLIPSOID = Homogeneous, isotropic ellipsoid.

"Lengths" SHPAR$_1$, SHPAR$_2$, SHPAR$_3$ in the x, y, z directions in the TF:

$$\left(\frac{x_{\mathrm{TF}}}{\mathrm{SHPAR}_1 d}\right)^2 + \left(\frac{y_{\mathrm{TF}}}{\mathrm{SHPAR}_2 d}\right)^2 + \left(\frac{z_{\mathrm{TF}}}{\mathrm{SHPAR}_3 d}\right)^2 = \frac{1}{4} \quad , \tag{37}$$

where d is the interdipole spacing.
The target axes are set to $\hat{\mathbf{a}}_1 = (1,0,0)_{\mathrm{TF}}$ and $\hat{\mathbf{a}}_2 = (0,1,0)_{\mathrm{TF}}$.
Target Frame origin = centroid of ellipsoid.
User must set NCOMP=1 on line 9 of `ddscat.par`.
A **homogeneous, isotropic sphere** is obtained by setting SHPAR$_1$ = SHPAR$_2$ = SHPAR$_3$ = diameter/d.

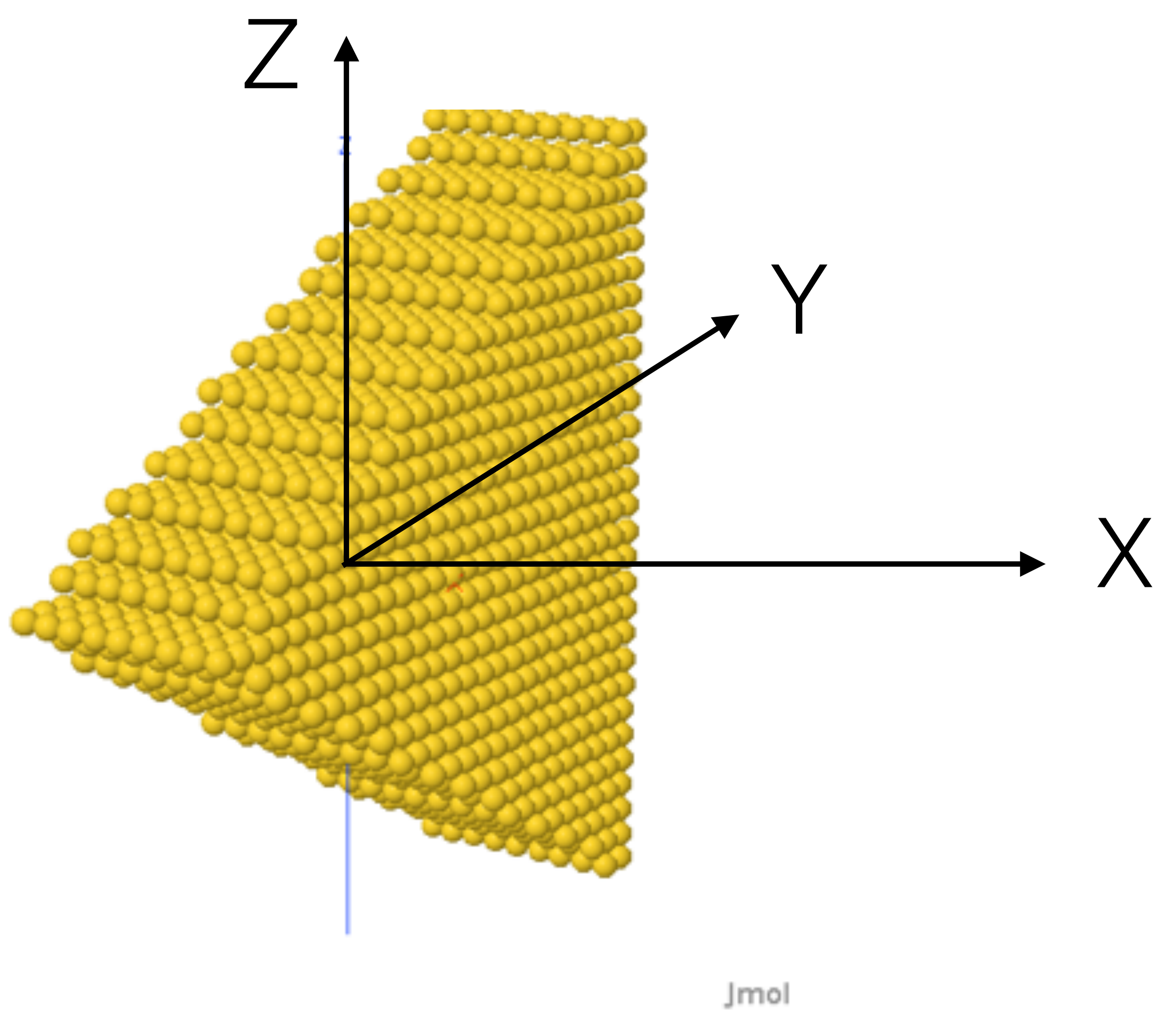


SHPAR1 = 20
SHPAR2 = 50
SHPAR3 = 20

Predefined Shape : TRNGLPRSM

21.25 TRNGLPRSM = Triangular prism of homogeneous, isotropic material

`SHPAR`$_1$, `SHPAR`$_2$, `SHPAR`$_3$, `SHPAR`$_4 = a/d, b/a, c/a, L/a$
The triangular cross section has sides of width a, b, c. L is the length of the prism. d is the lattice spacing. The triangular cross-section has interior angles α, β, γ (opposite sides a, b, c) given by $\cos\alpha = (b^2 + c^2 - a^2)/2bc$, $\cos\beta = (a^2 + c^2 - b^2)/2ac$, $\cos\gamma = (a^2 + b^2 - c^2)/2ab$. In the Target Frame, the prism axis is in the $\hat{x}$ direction, the normal to the rectangular face of width a is (0,1,0), the normal to the rectangular face of width b is $(0, -\cos\gamma, \sin\gamma)$, and the normal to the rectangular face of width c is $(0, -\cos\beta, -\sin\beta)$.



SHPAR1 = 30
SHPAR2 = 1
SHPAR3 = 1
SHPAR4 = 0.3

How is defined the nano-object geometry ?

The target is represented by an array of N dipoles, located on a cubic lattice with lattice spacing d.
The volume of the target is therefore :

$$\boxed{V = Nd^3}$$

We characterize the size of the target by the "effective radius"

$$\boxed{a_{\text{eff}} \equiv (3V/4\pi)^{1/3}}$$