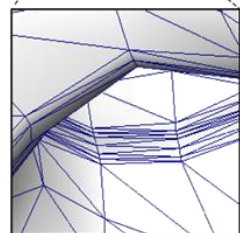
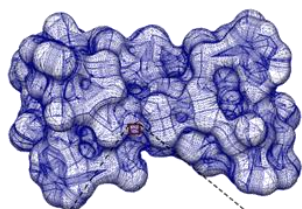
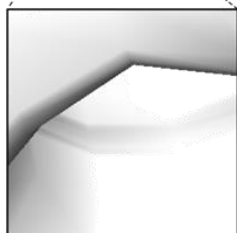
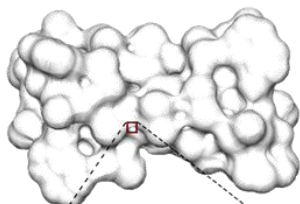


***Du ligand aux systèmes macromoléculaires :
visualisation interactive haute qualité grâce aux GPUs***

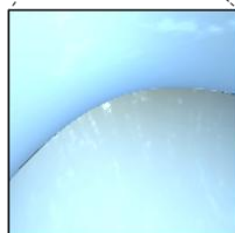
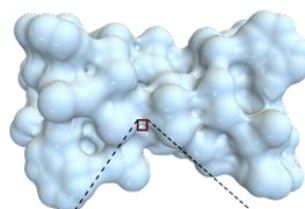
JOBIM 2010

**Matthieu Chavent (sous la direction de JP Nominé)
CEA, DIF, Arpajon**

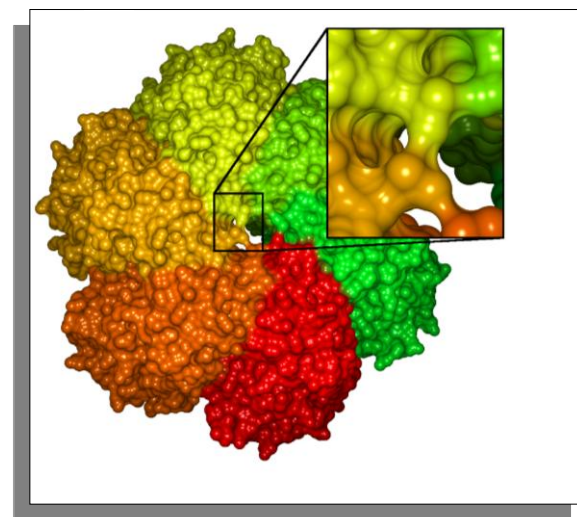
- Lancer de rayons sur GPU: un modèle «*vectériel*»
 - Précision au pixel près (plus ou moins rapide).

Gramicidin A (*side*)Triangulated
(with Wire Frame)

Triangulated



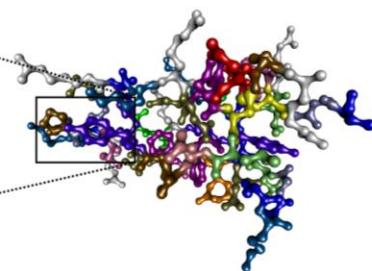
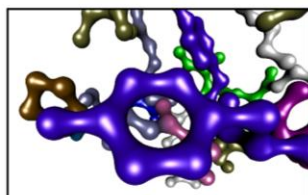
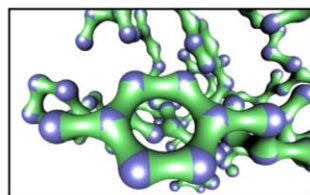
Ray Casted

• Molecular Surface²• Molecular Skin Surface¹

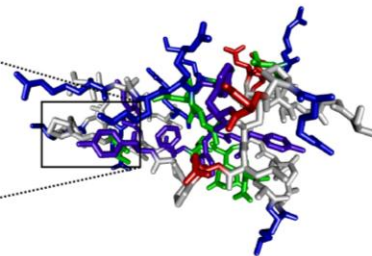
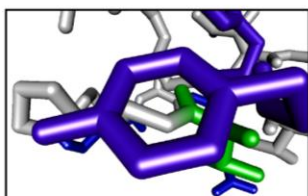
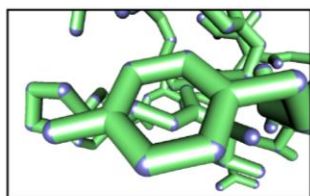
1. M. Chavent, B. Levy, and B. Maigret, *J Mol Graph Model* **27** (2), 209 (2008). 2. M. Krone, K. Bidmon, and T. Ertl, *IEEE Trans Vis Comput Graph* **15** (6), 1391 (2009).

Extension du lancer de rayon pour les représentations classiques: Ball & Stick, VdW...

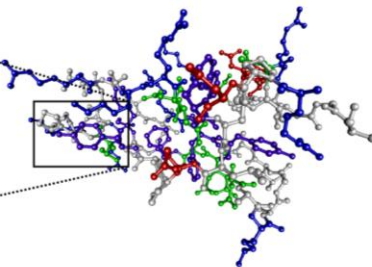
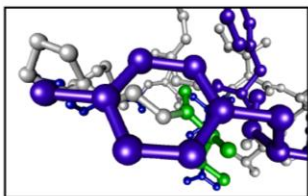
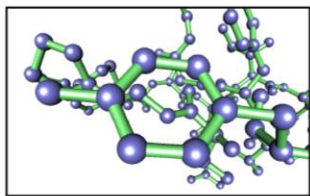
0 Les différents types de représentation:



HyperBalls

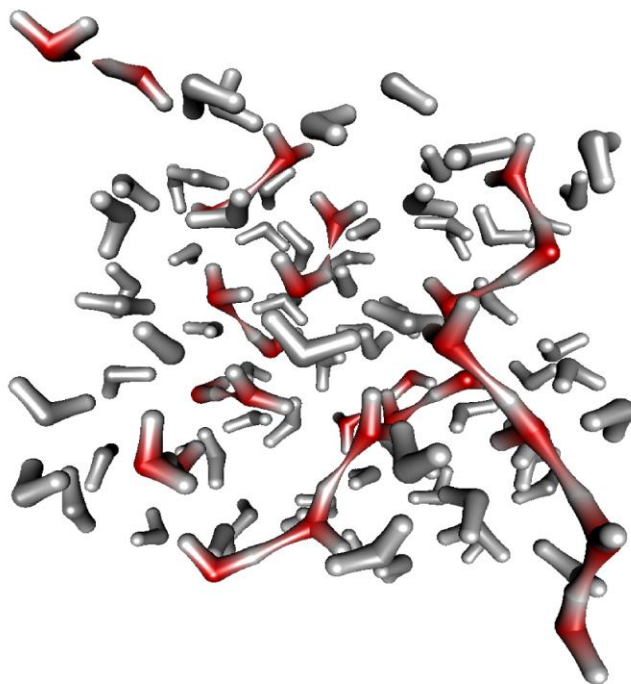
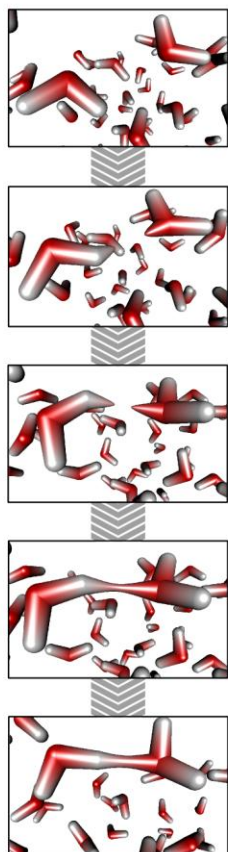


Licorice

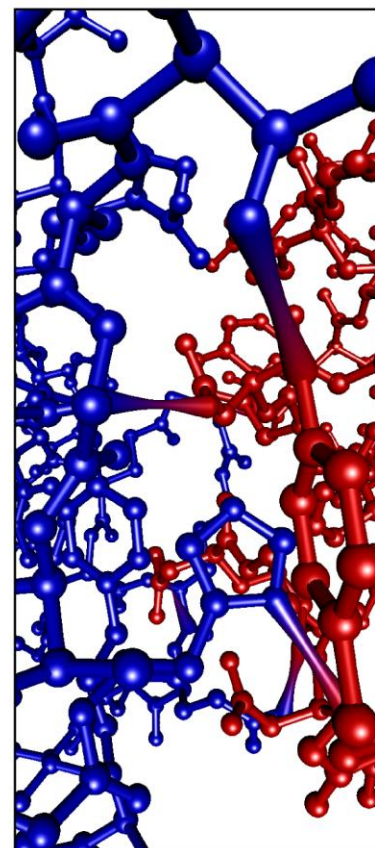


Ball & Stick

o Evolution temps réel des liaisons hydrogènes:

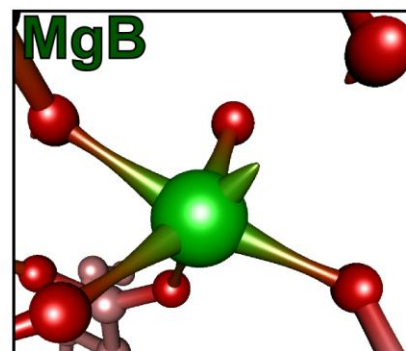
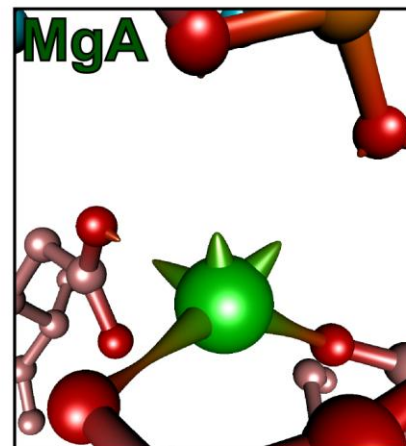
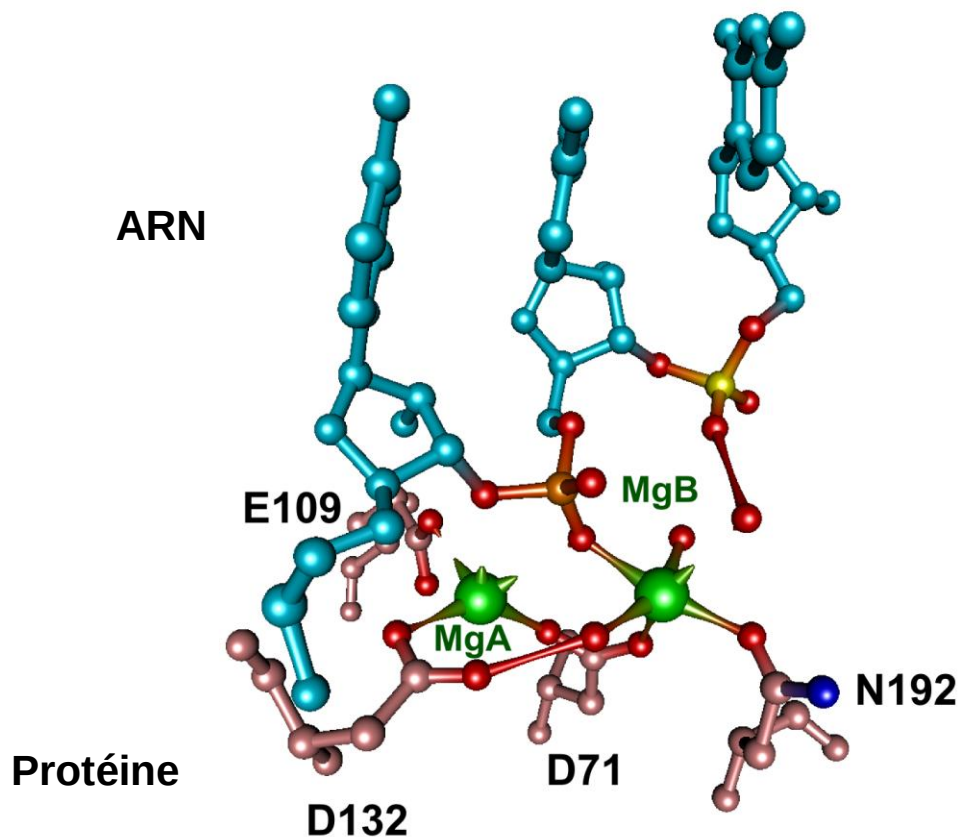


Entre molécules d'eau

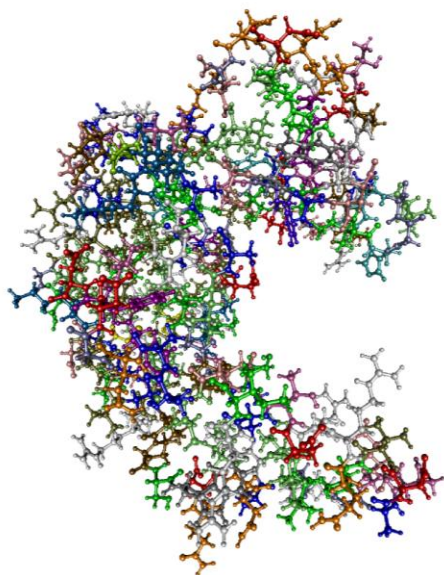


Entre protéines

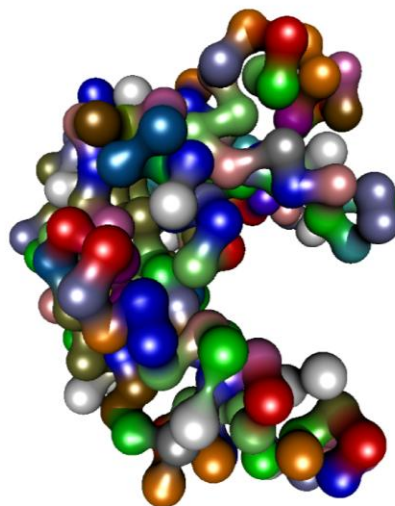
o Visualisation de coordination asymétrique :



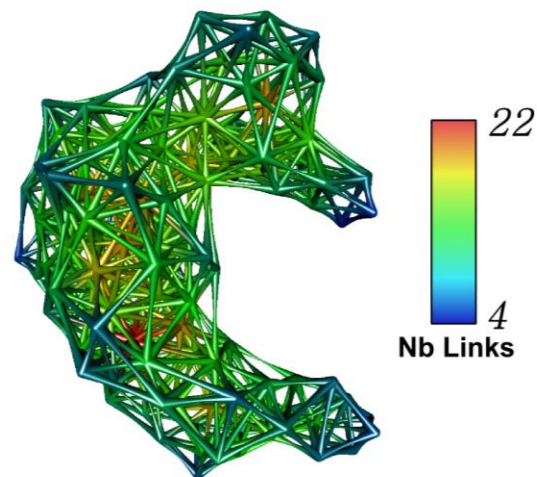
o Visualisation de modèles simplifiés :



Modèle « tout atome »

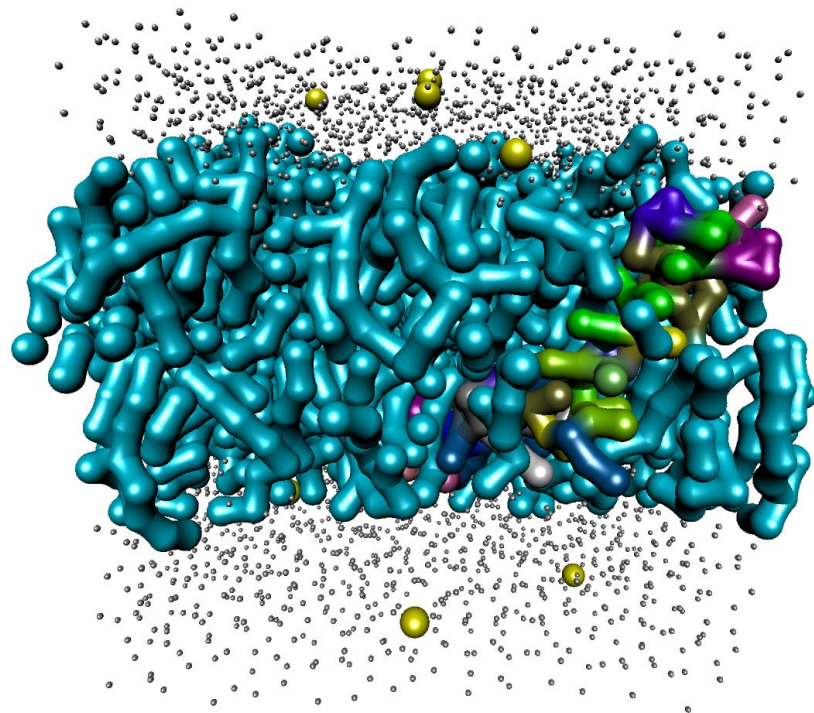
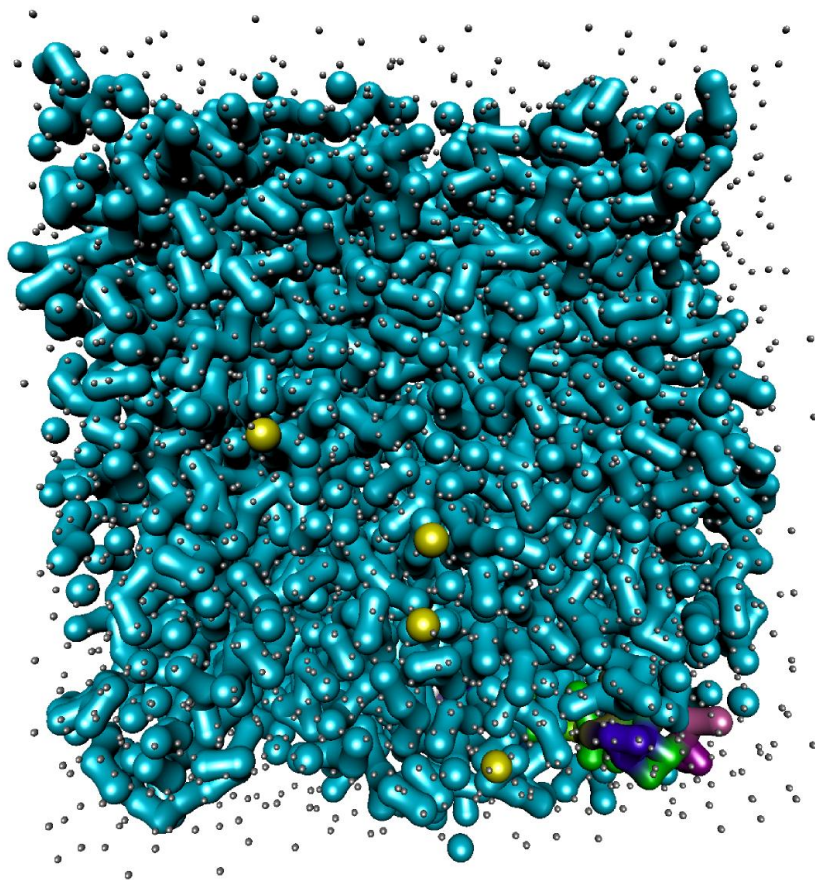


Modèle « gros grains »



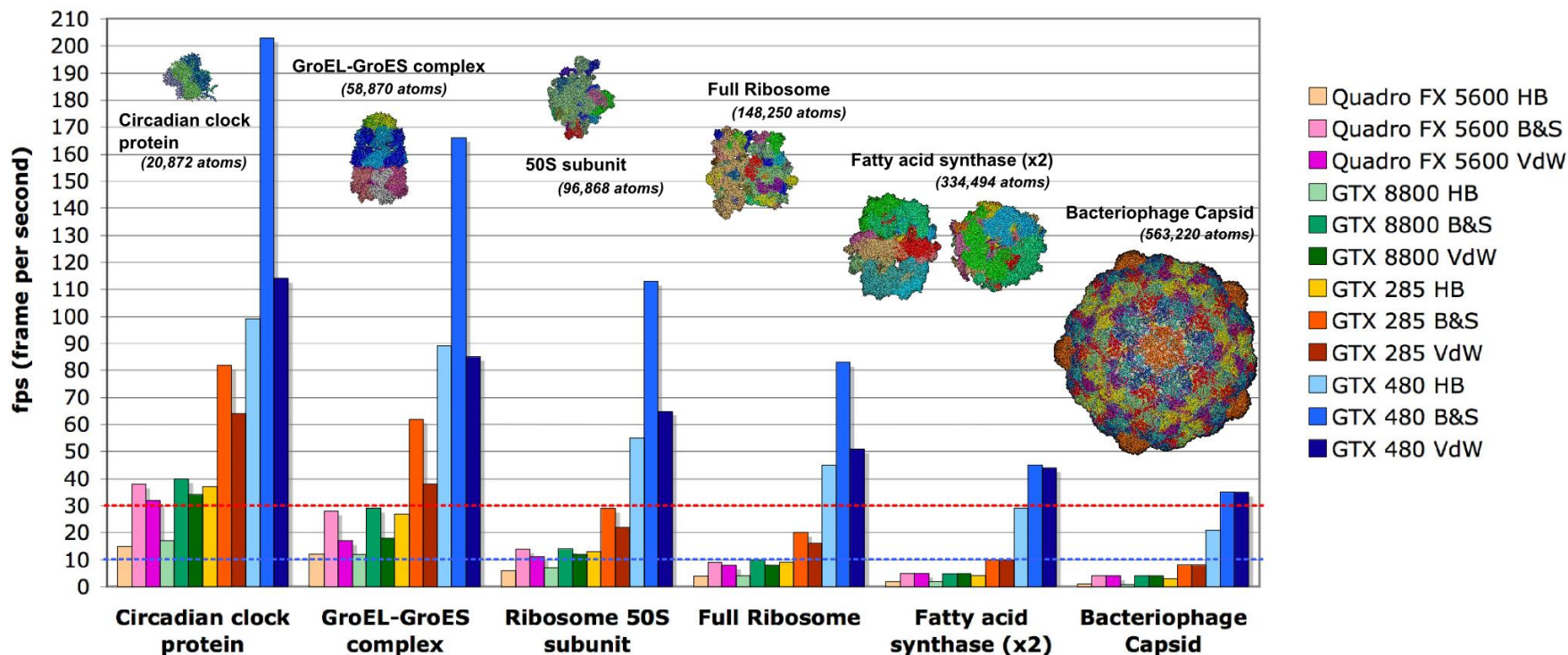
Modèle « réseau de ressorts »

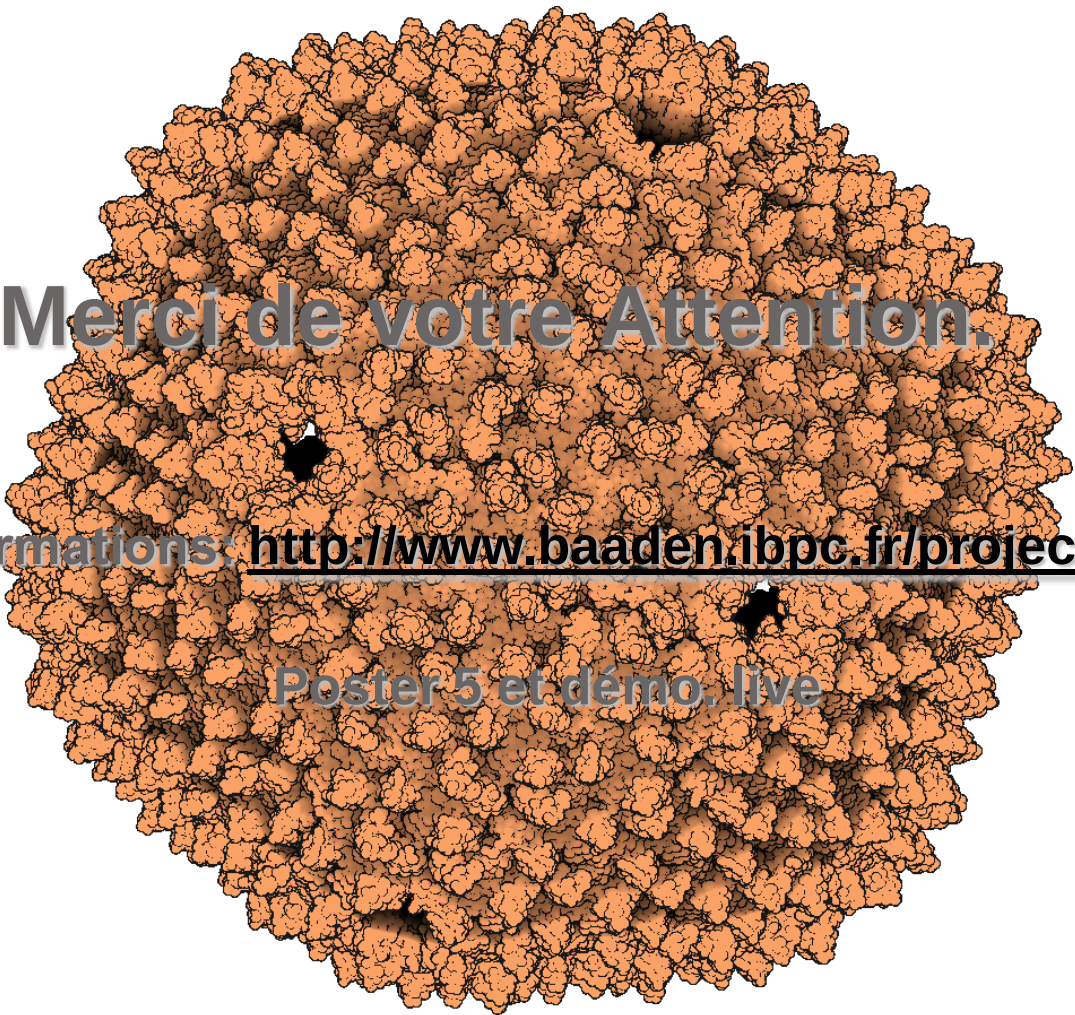
o Visualisation de modèles simplifiés :



Protéine dans une membrane + eau : modèle gros grains

○ Résultats : jeu de données statique





Merci de votre Attention.

Plus d'informations : <http://www.baaden.ibpc.fr/projects/fvnano/>

Poster 5 et démo. live

0 **Equipe MOAIS (INRIA, Grenobles)**

- 0 Antoine Vanel
- 0 Bruno Raffin

0 **LBT (IBPC, Paris)**

- 0 Alex Tek
- 0 Marc Baaden

0 **Equipe PRV (LIFO ,Orléans)**

- 0 Ahmed Turki
- 0 Sophie Robert
- 0 Sébastien Limet

0 **Equipe ALICE (INRIA, Nancy)**

- 0 Bruno Lévy

