Integrating simulated crystal growth into 3D modeling software

Comparison of simulated images (left) with experimental photomicrographies (middle and right). These simulated images are used as input for a supervised learning approach.

**Motivation:**

Technical protein crystallization is an attractive alternative to preparative chromatography as a main purification step of proteins in biotechnological processes. However, quantifying the crystallization behavior of various protein mutants remains a challenging problem. Light microscopy is non-invasive, but analysis is complicated by multiple factors. Protein crystals are completely transparent for normal backlight imaging techniques and are only visible through their refractive and reflective properties at the crystal borders, which might be only partially visible. Furthermore, high crystal density, desired scale invariance, and heterogeneous particles in crystallization buffers are additional challenges. In this project, the analysis of these photomicrographies is tackled via a machine learning approach to object detection based on Mask R-CNN-like approaches.

**Your tasks:**

- Integrating the existing simulation method of protein crystal growth into the BLENDER 3D modeling software with Python.
- Automate the high-quality rendering of crystallization processes in BLENDER for rapid generation of input-output pairs for supervised learning.
- Based on initial results, add varying noise contributions as regularization for training the network.

**Your profile:**

- Programming knowledge in Python.
- Experience with GitHub.
- Some Linux experience.

**Contact:**

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