Deep Learning-Based Foundation Model for Visual Analysis of Complex Particles

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COMPASS

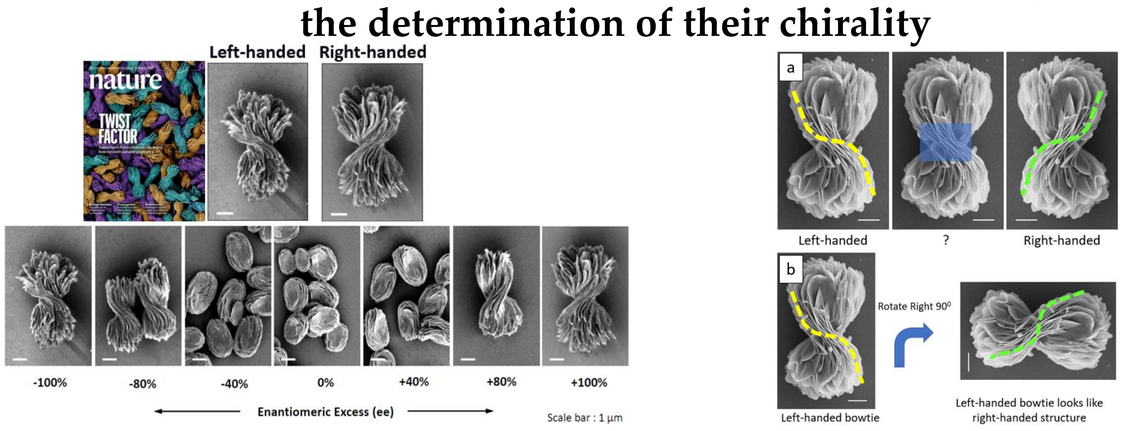
Motivation: build AI systems for complex particles through collaboration

Goals:

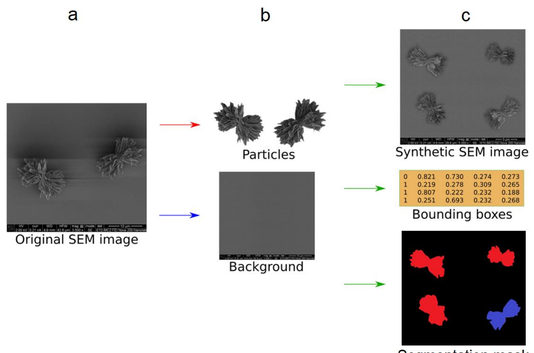
- Accelerate analysis of complex particles using Artificial Intelligence
- Develop new tools for 3D reconstruction of particle assemblies
- Create a Foundation Model for advanced visual analysis of complex particles

Chirality Analysis of Complex Particles using Deep Learning

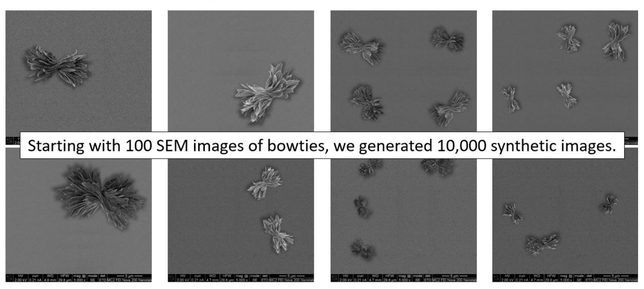
Self-assembled nanostructured bowties and challenges for the determination of their chirality



Structures detection using synthetic data



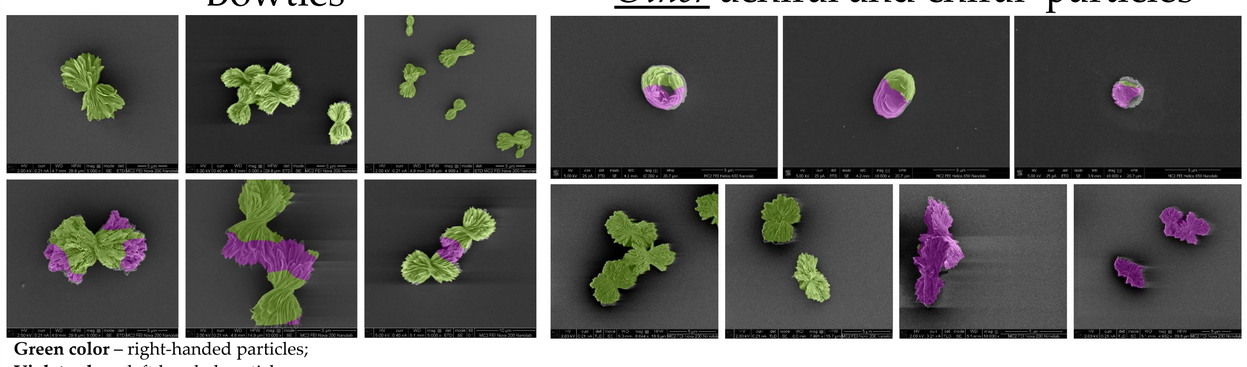
Idea: Generate large dataset of images using a small initial dataset of real images and train state-of-the-art model on it.



SegFormer-based semantic segmentation of complex particles

Bowties

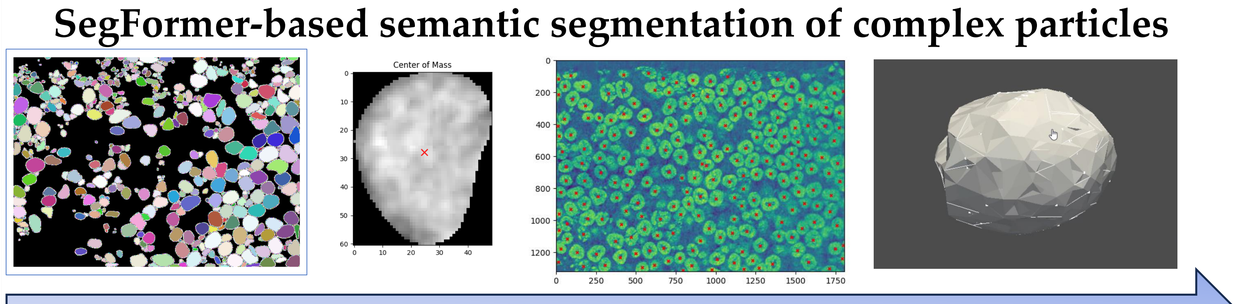
Other achiral and chiral particles



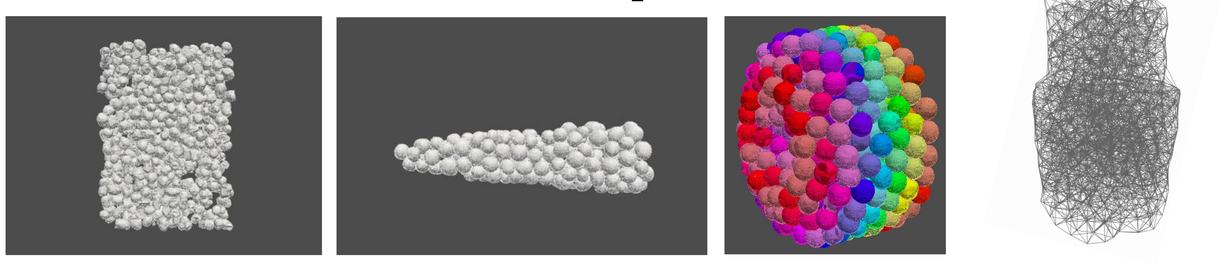
Green color – right-handed particles;
Violet color – left-handed particles.

Deep Learning-based 3D Reconstruction of Particles and their Ensembles

SegFormer-based semantic segmentation of complex particles



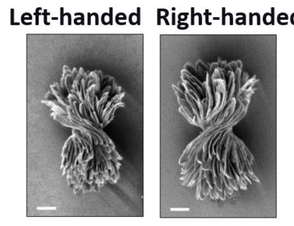
3D reconstructions of particle ensembles



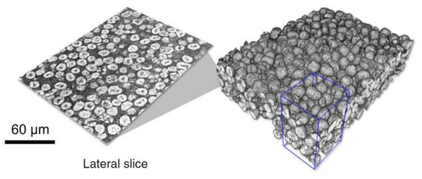
Prof. Qian Chen (University of Illinois at Urbana-Champaign) | Prof. Martin Thuo (North Carolina State University) | Prof. Ashley Bucsek (University of Michigan) | Particle centers graph

COMPASS Foundation Model for Visual Analysis of Complex Particles

Deep learning for electron microscopy



- Collect (plenty of) data
- Select model
- Train the model



Jiang Z. et al. *Nature communications*, 2020 , 11(1):2310.

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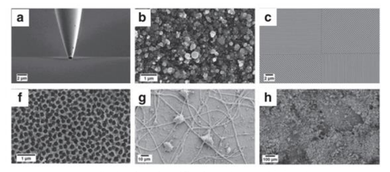
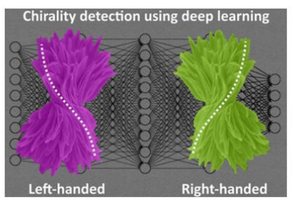


Aversa R. et al. *Scientific data*, 2018, 5(1):1-0.

Repeat!



How does Computer Science field solve such problem?

By developing Foundation Models

Advantages:
- ✓ Versatility
- ✓ Cost-Efficient
- ✓ Performance

Large-scale models that are pre-trained on vast amounts of data

Foundation Model for COMPASS: a greenfield project

Data — Complex particle data sharing among COMPASS participants

Community ⟷ **Compute**

Enhancement of COMPASS community connectivity

Collaboration through computational resources sharing

Conclusion

- Deep Learning algorithms can **identify** twisted bowtie-shaped microparticles with nearly **100% accuracy** and **classify** them as left- and right-handed with as high as **99% accuracy**.
- After training on bowtie particles with complex nanostructured features, the model can recognize ***other*** chiral shapes with different geometries without re-training for their specific chiral geometry with **93% accuracy**.
- **Deep learning-based particle segmentation is a powerful tool for 3D reconstruction of particles.**
- **COMPASS is a great community for developing Foundation Model for electron microscopy and beyond!**

References and Acknowledgements

1. Kumar, P., Vo, T., Cha, M., Visheratina, A., Kim, J.Y., Xu, W., Schwartz, J., Simon, A., Katz, D., Nicu, V.P. and Marino, E., 2023. Photonically active bowtie nanoassemblies with chirality continuum. Nature, 615(7952), pp.418-424.
2. Visheratina, A., Visheratin, A., Kumar, P., Veksler, M. and Kotov, N.A., 2023. Chirality Analysis of Complex Microparticles using Deep Learning on Realistic Sets of Microscopy Images. ACS nano, 17(8), pp.7431-7442.