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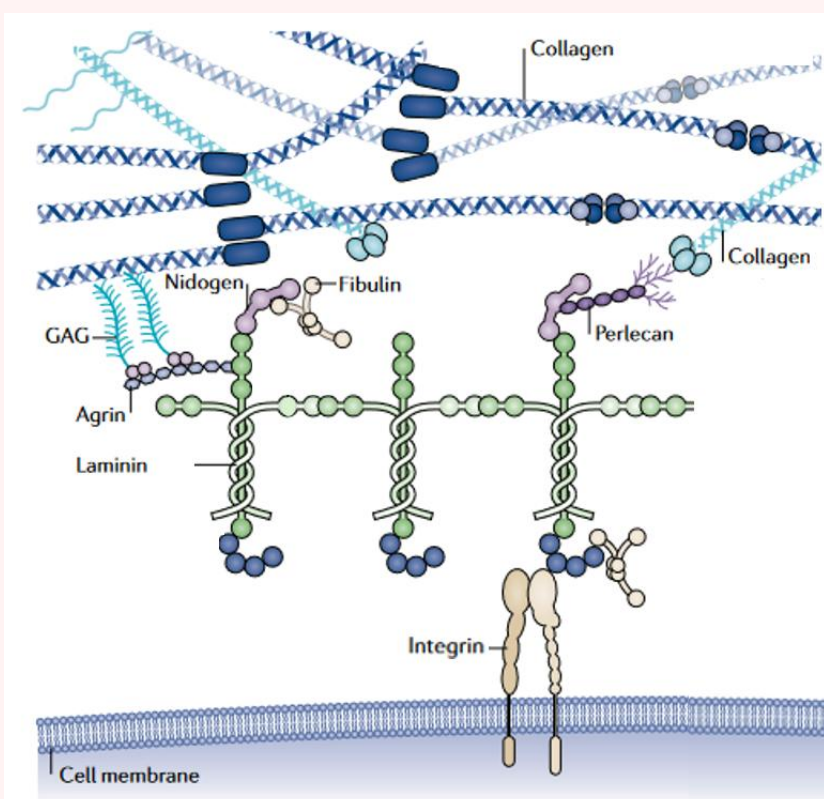
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INTRODUCTION

The extracellular matrix (ECM) is a complex three-dimensional network of macromolecules playing a central role in tissue organization, cell adhesion, migration and signaling. Alterations in the ECM composition and organization are associated with aging and numerous pathologies, including fibrosis, vascular diseases, cancer, and connective tissue disorders. However, due to the size and structural complexity of the ECM, its large-scale dynamics remain difficult to study with conventional atomistic simulations or experimental approaches alone.

This project focuses on the development and application of DURABIN (Developing Utilities for Nanometric Interactions in Biochemistry with augmented Reality), a mesoscopic multi-scale simulation framework developed in our laboratory (MEDyC) to study extracellular matrix organization. DURABIN relies on rigid-body dynamics and simplified geometrical representations of biomolecular domains to reduce computational cost while preserving the large-scale structural behavior of ECM components. This approach provides the simulation and visualization of supramolecular assemblies at an intermediate scale between atomistic molecular dynamics and microscopy. The project will build upon recent improvements introduced in the CHLORAINE extension, including enhanced conformational flexibility and the combination of physicochemical properties such as electrostatic and hydrophobic interactions.

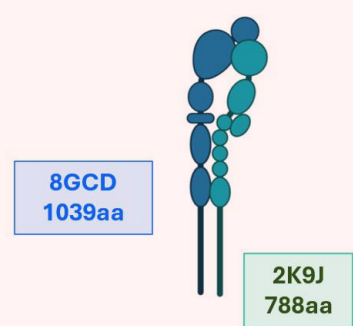
Why DURABIN?



Extracellular matrix adapted from Naylor et al.

- ✓ Complex Network of macromolecules
- ✓ Structural support, Cell adhesion and communication, Regulation of the cell behavior

Integrin – 1827 aa



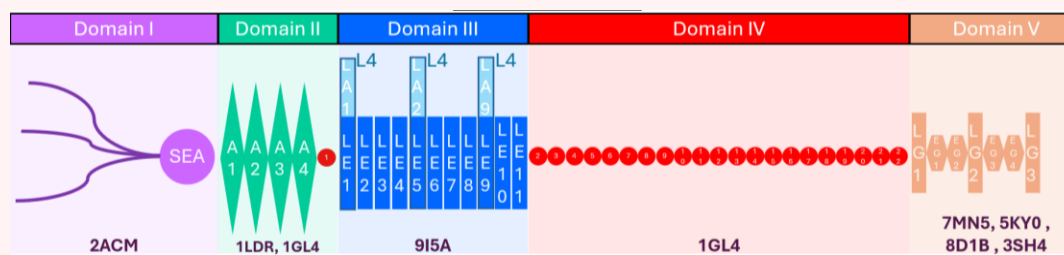
Collagen IV - α1α1α2



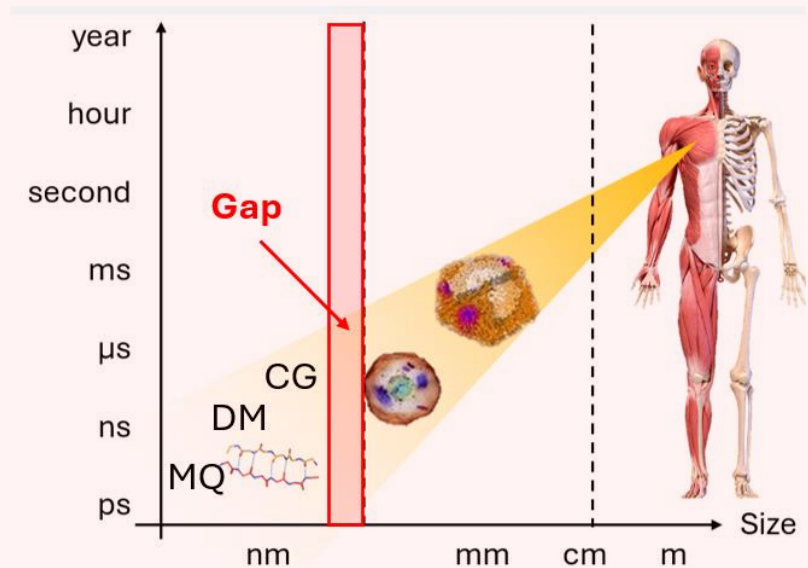
Laminin-111 - 6470 aa



Perlecan – 4391 aa

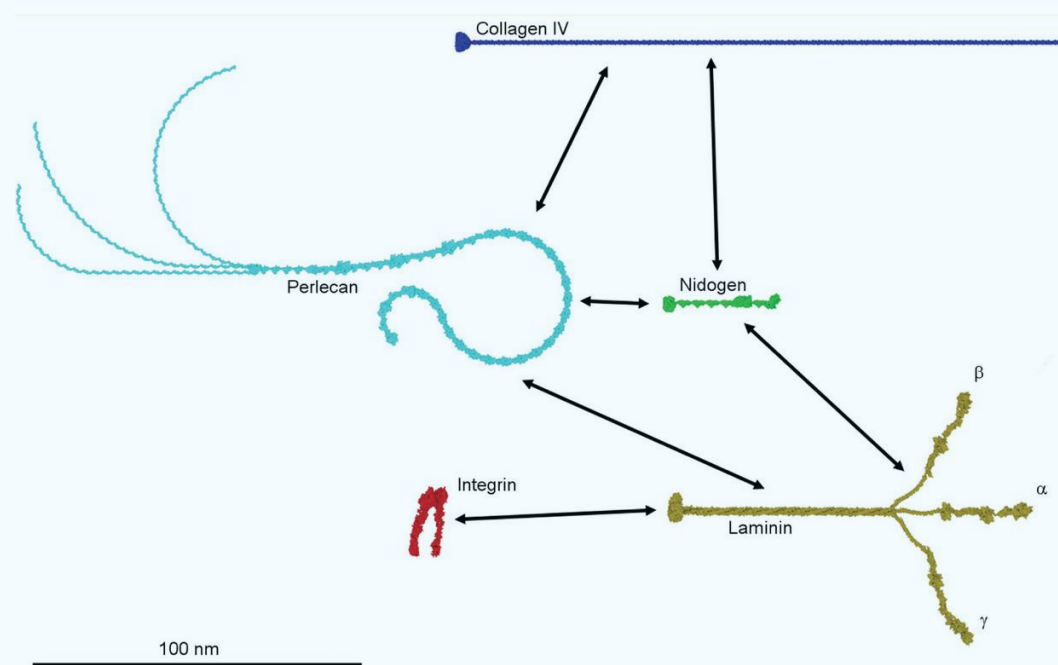
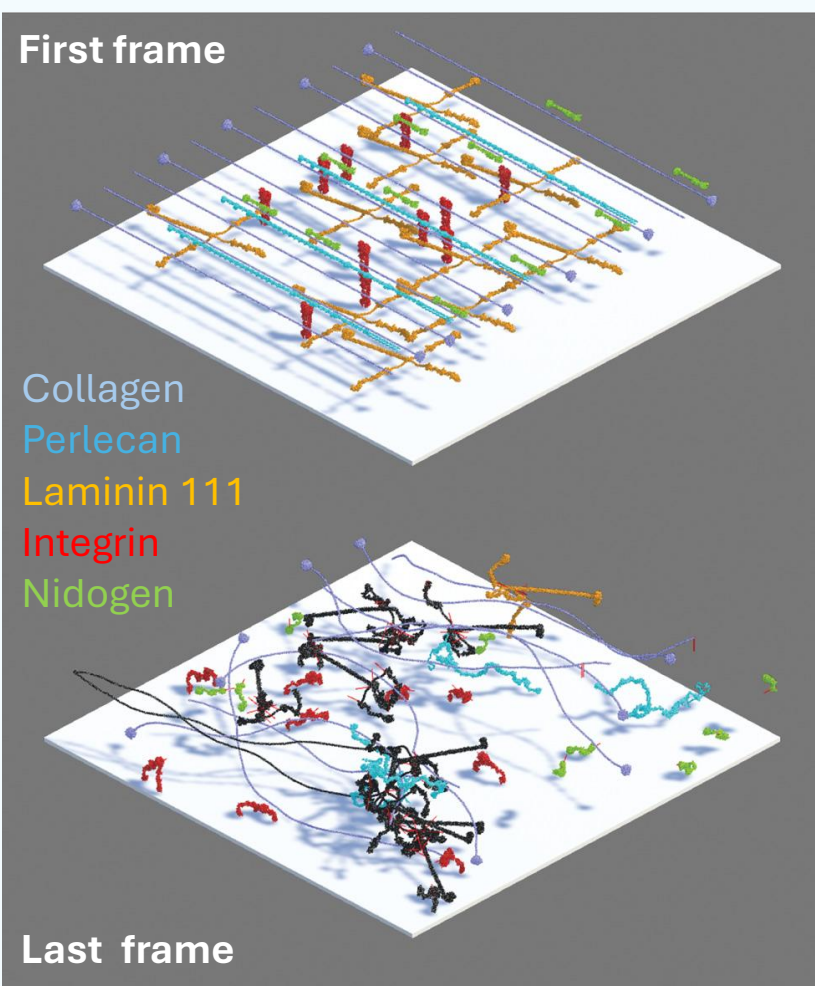


Nidogen – 1247 aa

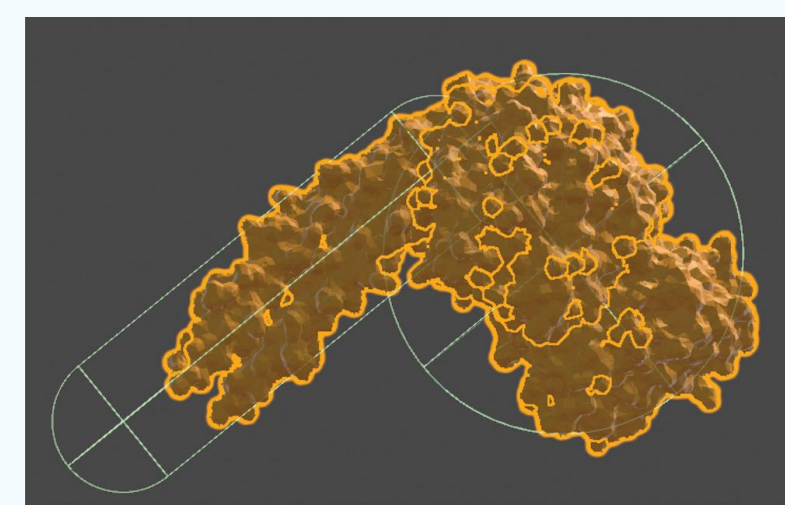


DURABIN

Developing Utilities for Nanometric Interactions in Biochemistry with augmented Reality¹



The proportions between the components are maintained

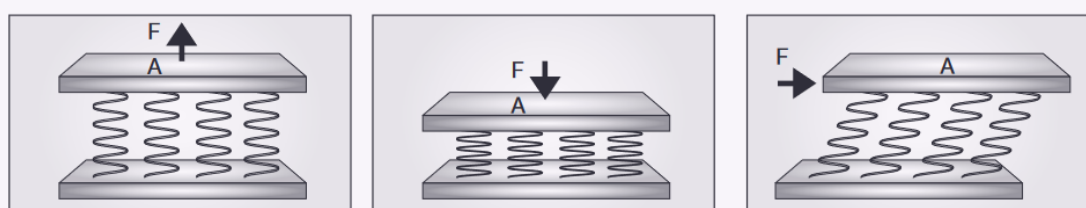


Globular domain of the laminin*

Colliders - joints

PERSPECTIVES

Three phenomena:



Extension

Compression

Shear Stress

Composition in pathologies:

	Collagen	Nidogen	Laminin-111
#1	45 IV 45 XVIII	10	
#2	30 XVIII	10	60

- ✓ Cancer – degradation of the laminin-111
- ✓ Cancer – degradation of the collagen IV

REFERENCES

Wong, Hua, PrévotEAU-Jonquet, Jessica, Baud, Stéphanie, Dauchez, Manuel and Belloy, Nicolas. "Mesoscopic Rigid Body Modelling of the Extracellular Matrix Self-Assembly" *Journal of Integrative Bioinformatics*, vol. 15, no. 2, 2018, pp. 20180009.

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