The Spherical Design Algorithm in the Numerical Simulation of Fibre-Reinforced Biological Tissues

Melania Carfagna[1], Alfio Grillo[1]

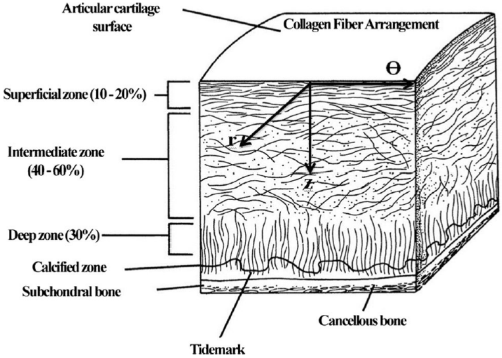
[1]DISMA *G.L.Lagrange* Politecnico di Torino

October the 13^{th}, 2016
Comsol Conference - Munich

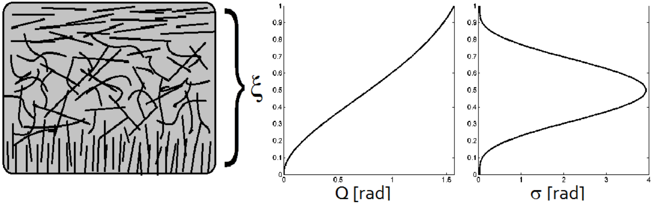
COMSOL CONFERENCE
2016 MUNICH

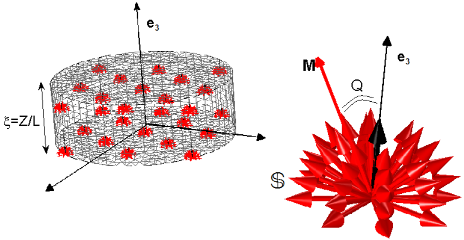
Articular Cartilage

- Living Cells (proteoglycans,chondrocytes) constituting the ECM.
- Fibres of Collagen statistically distributed
- Fluid (mainly water) passing through and escaping from the tissue



Fibres Distribution



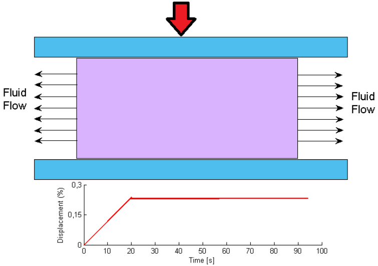


$$\hat{\Psi}(\xi,\Theta) = \frac{1}{\mathcal{Z}(\xi)} \exp\left(-\frac{[\Theta - Q(\xi)]^2}{2[\sigma(\xi)]^2}\right)$$

$$\mathbb{S}^2_X\mathcal{B} := \{\boldsymbol{M} \in T_X\mathcal{B} : \ \|\boldsymbol{M}\| = 1\}$$

$$\boldsymbol{M} = \sin(\Theta)\cos(\Phi)\boldsymbol{\mathcal{E}}_1 + \sin(\Theta)\sin(\Phi)\boldsymbol{\mathcal{E}}_2 + \cos(\Theta)\boldsymbol{\mathcal{E}}_3$$

Mechanical Behaviour - Unconfined Compression



$$\begin{cases} \dot{J} + \mathrm{Div}\left(-\hat{\boldsymbol{K}}(\boldsymbol{F})\,\mathrm{Grad}\,p\right) = 0 \\ \mathrm{Div}\left(-Jp\,\boldsymbol{g}^{-1}\boldsymbol{F}^{-\mathrm{T}} + \hat{\boldsymbol{P}}_{\mathrm{sc}}(\boldsymbol{F})\right) = \boldsymbol{0} \end{cases}$$

$$\hat{\boldsymbol{K}}(\boldsymbol{F}) = \boldsymbol{K}_{\mathrm{i}}(\boldsymbol{C},\xi) + \alpha(\boldsymbol{C},\xi)\hat{\boldsymbol{Z}}(\boldsymbol{C})$$

$$\boldsymbol{Z} = \hat{\boldsymbol{Z}}(\boldsymbol{C}) = \int_{\mathbb{S}^2\mathcal{B}} \Psi(\boldsymbol{M})\frac{\boldsymbol{M}\otimes\boldsymbol{M}}{I_4(\boldsymbol{C},\boldsymbol{M})}.$$

$$\hat{\boldsymbol{P}}_{\mathrm{sc}}(\boldsymbol{F}) = \boldsymbol{P}_{\mathrm{i}}(\boldsymbol{F}) + \boldsymbol{F}\boldsymbol{S}_{\mathrm{a}}$$

$$\boldsymbol{S}_{\mathrm{a}} = 2\phi_{1\mathrm{sR}}c\int_{\mathbb{S}^2\mathcal{B}} \Psi(\boldsymbol{M})\mathcal{H}(I_4-1)[I_4-1]\boldsymbol{A}.$$

in which $\boldsymbol{A} = \boldsymbol{M}\otimes\boldsymbol{M}$, $I_4 = \boldsymbol{C}:\boldsymbol{A}$.

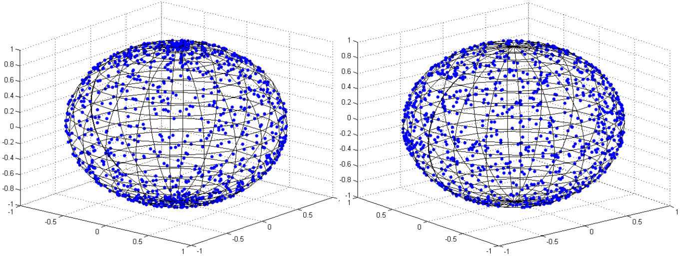
The Spherical Design Algorithm

Let f be any (scalar, vector, or tensor) function defined over $\mathbb{S}^2\mathcal{B}$.
Then $f(X, \boldsymbol{M}) = \hat{f}(X, \Theta, \Phi)$ with $(\Theta, \Phi) \in \mathcal{D} = [0, \pi] \times [0, 2\pi]$.

$$\int_{\mathbb{S}^2\mathcal{B}} f(\boldsymbol{M}) = \iint_{\mathcal{D}} \hat{f}(\Theta, \Phi) \sin(\Theta) \mathrm{d}\Theta \mathrm{d}\Phi$$

$$\iint_{\mathcal{D}} \hat{f}(\Theta, \Phi) \sin(\Theta) \mathrm{d}\Theta \mathrm{d}\Phi \simeq \frac{4\pi}{N} \sum_{i=1}^{m} \sum_{j=1}^{n} \hat{f}(\mathcal{X}_{ij})$$

with $\mathcal{X}_{ij} = (\Theta_i, \Phi_j) \in \mathcal{D}$, with $i = 1, \ldots, m$ and $j = 1, \ldots, n$, $N = mn$.

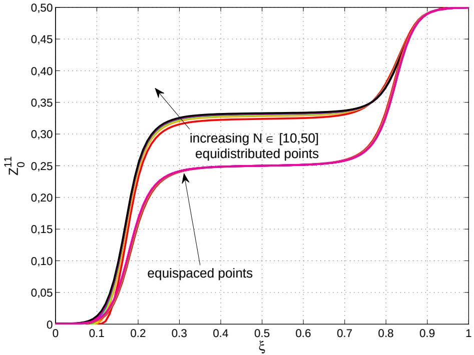


The Proper Choice of the Integration Points

$$(\mathbf{Z}_0)^{11} = (\mathbf{Z}_0)^{22} = \pi \int_0^{\pi} \hat{\Psi}(\xi,\Theta)[\sin(\Theta)]^3 \mathrm{d}\Theta,$$

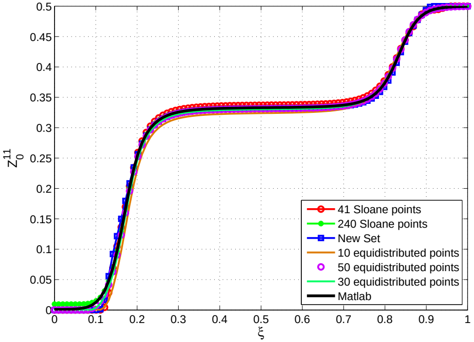
$$(\mathbf{Z}_0)^{12} = (\mathbf{Z}_0)^{13} = (\mathbf{Z}_0)^{23} = 0,$$

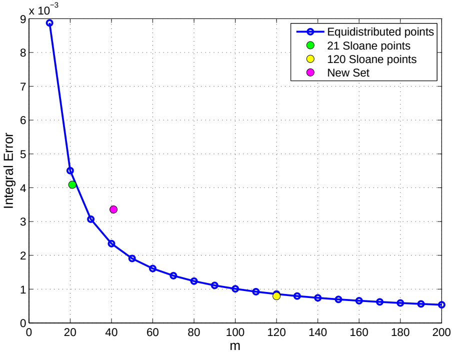
$$(\mathbf{Z}_0)^{33} = 1 - 2(\mathbf{Z}_0)^{11}.$$

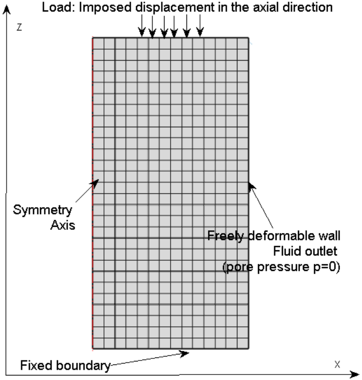


The Proper Choice of the Integration Points

$$(\mathbf{Z}_0)^{11} = (\mathbf{Z}_0)^{22} = \pi \int_0^{\pi} \hat{\Psi}(\xi, \Theta)[\sin(\Theta)]^3 d\Theta,$$
$$(\mathbf{Z}_0)^{12} = (\mathbf{Z}_0)^{13} = (\mathbf{Z}_0)^{23} = 0,$$
$$(\mathbf{Z}_0)^{33} = 1 - 2(\mathbf{Z}_0)^{11}.$$







$$w(t) = -0.2L\frac{t}{T}.$$

$$\begin{cases} \dot{J} + \mathrm{Div}\left(-\hat{\boldsymbol{K}}(\boldsymbol{F})\,\mathrm{Grad}\,p\right) = 0 \\ \mathrm{Div}\left(-Jp\,\boldsymbol{g}^{-1}\boldsymbol{F}^{-\mathrm{T}} + \hat{\boldsymbol{P}}_{\mathrm{sc}}(\boldsymbol{F})\right) = \boldsymbol{0} \end{cases}$$

$$\begin{aligned} &\chi^3 = H + w, && \boldsymbol{Q}.\boldsymbol{E}_3 = 0, && \forall X \in \Gamma_{\mathrm{u}} \\ &-p = 0, && \boldsymbol{P}.\boldsymbol{N} = \boldsymbol{0}, && \forall X \in \Gamma_{\mathrm{w}} \\ &\chi^3 = 0, && \boldsymbol{Q}.(-\boldsymbol{E}_3) = 0, && \forall X \in \Gamma_{\mathrm{l}} \end{aligned}$$

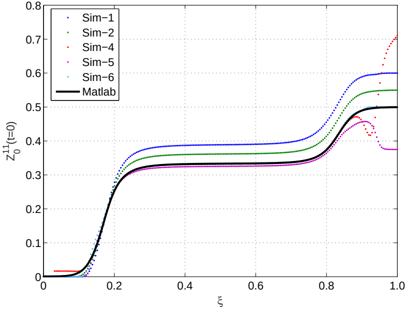
Benchmark Tests

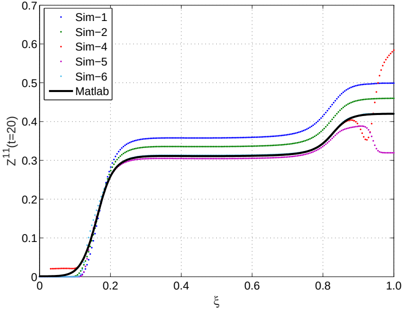
Name	Performed integration	N
Sim-1	SDA	50 equidistributed
Sim-2	SDA	200 equidistributed
Sim-3	Matlab Integration, external call to Matlab	//
Sim-4	SDA	21 Sloane points
Sim-5	SDA	120 Sloane points
Sim-6	SDA	41, $(\Theta, \Phi) \in \mathcal{I} \times \mathcal{J}$

$$\Theta \in \mathcal{I} = \left\{0, \frac{\pi}{6}, \frac{\pi}{4}, \frac{\pi}{3}, \frac{2\pi}{5}, \frac{\pi}{2}\right\},$$

$$\Phi \in \mathcal{J} = \left\{0, \frac{\pi}{4}, \frac{\pi}{2}, \frac{3\pi}{4}, \pi, \frac{5\pi}{4}, \frac{3\pi}{2}, \frac{7\pi}{4}\right\}.$$

Results - Radial Permeability

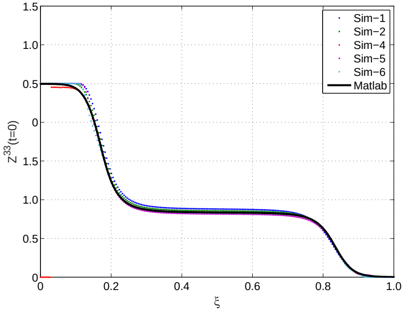


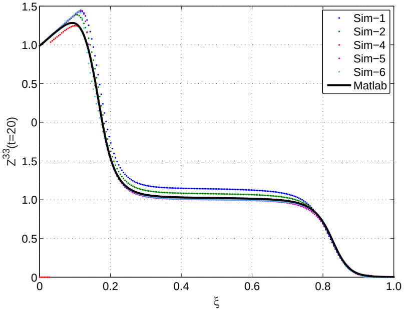


	Sim-1	Sim-2	Sim-4	Sim-5	Sim-6
Comp. Time	5 min 15 s	≈ 40 s	55 s	2 min 20 s	≈ 30 s
Memory [Gb]	2.52	2.54	2.53	1.44	1.21

Sim-3 Computational time: 3 h 40 min
Sim-3 Memory: 2.4 Gb

Results - Axial Permeability





	Sim-1	Sim-2	Sim-4	Sim-5	Sim-6
Comp. Time	5 min 15 s	$\approx$ 40 s	55 s	1 min 20 s s	18 s
Memory [Gb]	2.52	2.54	2.53	1.44	1.21

Results - Stress

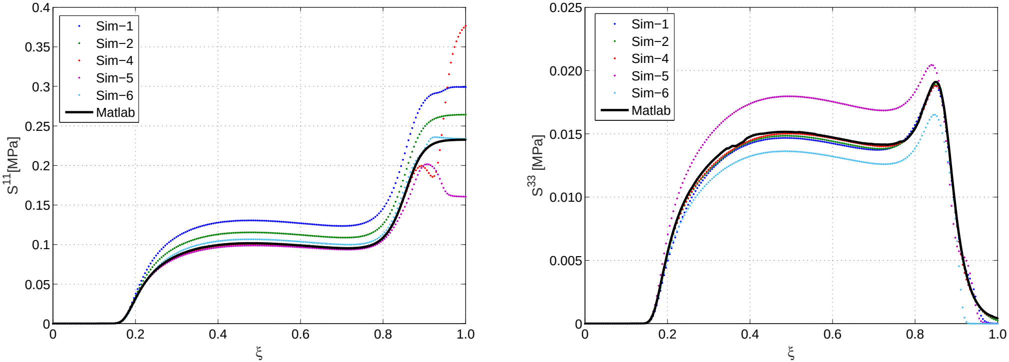


Figure: Radial (left) and Axial (right) stress components related to fibres

Conclusions

- If the quadrature points are properly chosen, an internal implementation of the SDA is in general preferable to an external Matlab call.
- To validate the point set $\mathcal{I} \times \mathcal{J}$ for a more general computational and mathematical setting, we need to test it on a wider range of benchmark problems and constitutive laws.

Some Citations

- Aspden, R.M., Hukins, D.W.L.: Collagen organization in articular cartilage, determined by X-ray diffraction, and its relationship to tissue function, *Proc. R. Soc. B*, 212:299–304, 1981.
- Carfagna, M., Grillo, A., Federico, S., The Spherical Design Algorithm in the numerical simulation of biological tissues with statistical fibre-reinforcement, submitted.
- Hardin, R.H., Sloane, N.J.A.: McLaren's Improved Snub Cube and Other New Spherical Designs in Three Dimensions, *Discrete and Computational Geometry*, 15:429–441, 1996.
- Delsarte, P., Goethals, J.M., Seidel, J.J.: Spherical codes and designs, *Geometriae Dedicata*, 6:363–388, 1977.
- Spherical t-designs: http://neilSloane.com/sphdesigns/dim3/

Thank You For Your Kind Attention