Shape design of a polymer microstructure for bones

joint work with M. Rumpf and S. Simon

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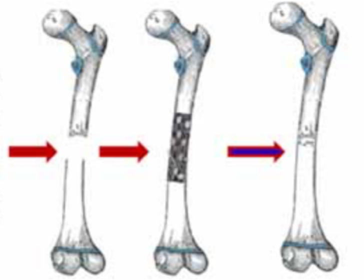
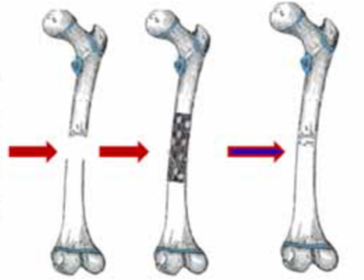
Context

- Critical sized bone defects due to trauma, osteoporosis or osteosarcoma comprise a major reason for disability.
- Despite many issues, autograft is still the gold standard of treatment.
- A number of substitutes are being explored.



Ideal Scaffold

- Biocompatible.
- Bioresorbable.
- Provides mechanical stability during regeneration process.
- Does not prevent osteogenesis.



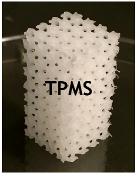
Comparison of current strategies

		Osteo-conduction	Osteo-induction	Osteo-genesis	Osteo-integration	Structural support	Disadvantages
Autologous Bone	Autologous Cancellous	+++	+++	+++	+++	–	Limited availability and donor site morbidity
Allogeneic Bone	Allogeneic Cancellous	+	+	–	++	–	Risk of disease transmission and immune reaction
	DBM	+	++	–	++	–	Variable osteoinductivity associated with donors and processing methods
Synthetic Substitutes	Calcium sulfate	+	–	–	++	+	Rapid resorption,osteoconductive only
	Hydroxyapatite	+	–	–	–	++	Slow resorption,osteoconductive only
	Calcium phosphate ceramic	+	–	–	+	++	Osteoconductive only
	Calcium phosphate cement	+	–	–	+	+	Osteoconductive only
	Bioactive glass	+	–	–	–		Bioactive osteoconductive only
	PMMA	–	–	–	–	+++	Inert, exothermic,monomer-mediate toxic

Adapted from: Bhatt, R. A., & Rozental, T. D. (2012). Bone graft substitutes. Hand Clinics, 28(4), 457–468. http://doi.org/10.1016/j.hcl.2012.08.001

Additively manufactured scaffolds

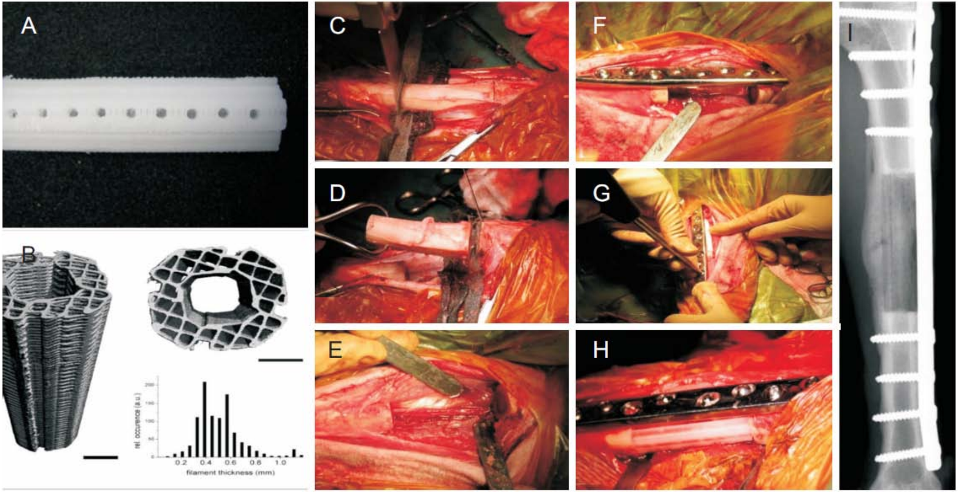
- Made from Polycaprolactone (PCL).
- Flexibility, patient customization.
- Conventional raster-angle scaffolds: very low resistance to shear, torsion, compression.
- Triply periodic minimal surfaces (TMPS): newer approach.
- Generally, polymer scaffolds are fairly soft, so one would want to increase their stiffness.



Shape optimization

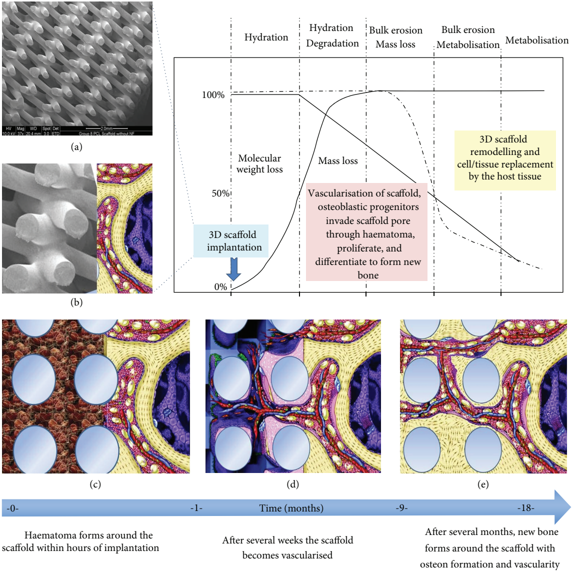
Numerical optimization of additively manufactured scaffolds seems like the natural next step in their design.

Surgical procedure



Henkel et. al., Bone Research (2013)

Bulk erosion



Henkel et. al., Bone Research (2013)

Shape optimization

Setting

$\Omega = [0,1]^3$ (scaled) micro cell. For a material $m \in \{\mathrm{b(one)}, \mathrm{p(olymer)}\}$, $\chi^m : \Omega \to \{0,1\}$ describes a (periodic) material distribution. The effect of bulk erosion yields $\chi^{\mathrm{b}} = 1 - \chi^{\mathrm{p}}$, so we set $\chi^{\mathrm{p}} = \chi$. We assume isotropic linearly elastic materials.

State equations

Given a material distribution $\chi^m : \Omega \to \{0,1\}$ the homogenized elasticity tensor C_*^m in a certain direction $A^m \in \mathbb{R}^{3\times 3}_{\mathrm{sym}}$ (or the elastic energy $E^m_{A^m}$ for the given load A^m) are

$$\begin{aligned} E^m_{A^m}[\chi^m] &= C_*^m[\chi^m]A^m : A^m \\ &= \min_{\tilde{u}^m \in H^1_\#(\Omega,\mathbb{R}^3)} \int_\Omega \chi^m C^m \left(A^m + \varepsilon(\tilde{u}^m)\right) : \left(A^m + \varepsilon(\tilde{u}^m)\right) \mathrm{d}x. \end{aligned}$$

Optimization problem

Cost functional

- We want the material to be mechanically stable and therefore we maximize the elastic energy.
- The scaffold and the regenerated bone will be subject to a number of different loading conditions A_j^m, all of which should be stable, so we maximize the minimum by using a weighting function $g(\{E\}_j) = \left(\sum_j \frac{1}{E_j^p}\right)^{\frac{1}{p}}$.
- We also take the minimum of the energy of the scaffold and the bone.
- This yields a compliance cost of

$$J_{\mathrm{c(ompliance)}}[\chi] = \max\left(g^{\mathrm{b}}(\{E^b_{A_j^b}\}_{j=1}^N), g^{\mathrm{p}}(\{E^{\mathrm{p}}_{A_j^{\mathrm{p}}}\}_{j=1}^N)\right).$$

- We add a surface area penalty $c_{\mathrm{Per}}\,\mathrm{Per}(\chi)$.

We use a standard phase field approximation for χ and regularize the max as $\max_\eta(x, y) = \frac{1}{2}(x + y + \sqrt{|x - y|^2 + \eta})$.

Shape derivative

We have to compute

$$\delta_v J_c(v)[\hat{v}] = \partial_v J_c(v, \tilde{u}_l^m)[\hat{v}] + \sum_{m \in \{b,p\}} \sum_j \partial_{\tilde{u}_j^m} J_c(v, \tilde{u}_l^m) \partial_v \tilde{u}_j^m(v)[\hat{v}],$$

where the second term can be computed using the adjoint problem.

Discretization

Using piecewise linear, continuous basis functions on a cuboid mesh, Lagrange multipliers for vanishing average conditions $\tilde{u}_j$ and center of mass for χ. We use an ersatz material to fill the empty space and a quasi-Newton (BGFS) method to approximate the optimizer.

Numerical results

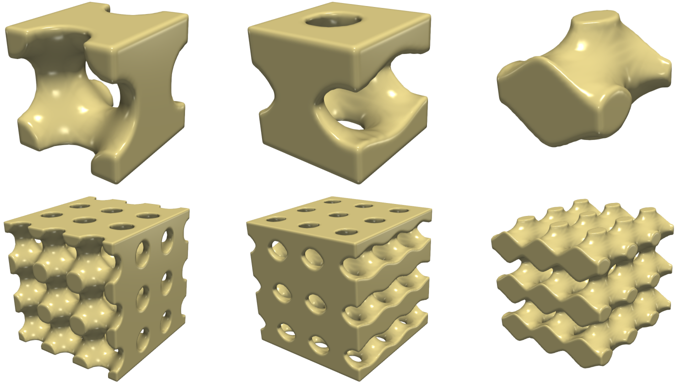
Loading conditions

We consider various combinations of the following loads:

$$A_1 = \begin{pmatrix} \beta & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},\ A_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \beta & 0 \\ 0 & 0 & 0 \end{pmatrix},\ A_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \beta \end{pmatrix},$$

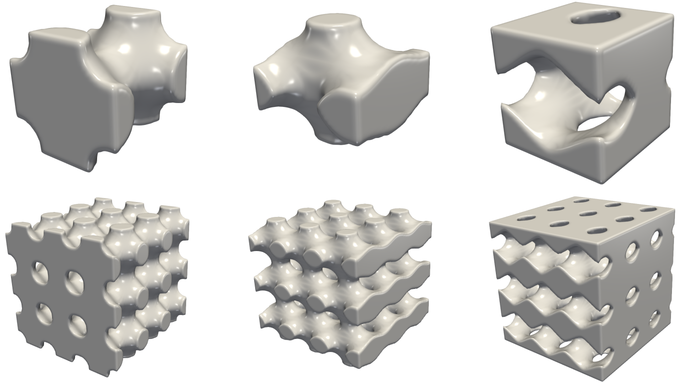
$$A_4 = \begin{pmatrix} 0 & \beta & 0 \\ \beta & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},\ A_5 = \begin{pmatrix} 0 & 0 & \beta \\ 0 & 0 & 0 \\ \beta & 0 & 0 \end{pmatrix},\ A_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \beta \\ 0 & \beta & 0 \end{pmatrix}.$$

Results in the symmetric case (polymer)



	B	P	B	P	B	P
Load 1	0.028858	0.028138	0.028858	0.028138	0.040894	0.040897
Load 2	0.028304	0.028651	0.028304	0.028651	0.021201	0.021219
Load 3	0.028304	0.028651	0.028304	0.028651	0.021218	0.021202
Load 4	0.024839	0.024922	0.024839	0.024922	0.029377	0.029381
Load 5	0.024839	0.024922	0.024839	0.024922	0.029382	0.029376
Load 6	0.024839	0.024918	0.024839	0.024918	0.010773	0.010773
vol	0.49975	0.50025	0.49975	0.50025	0.49999	0.50001

Results in the symmetric case (bone)



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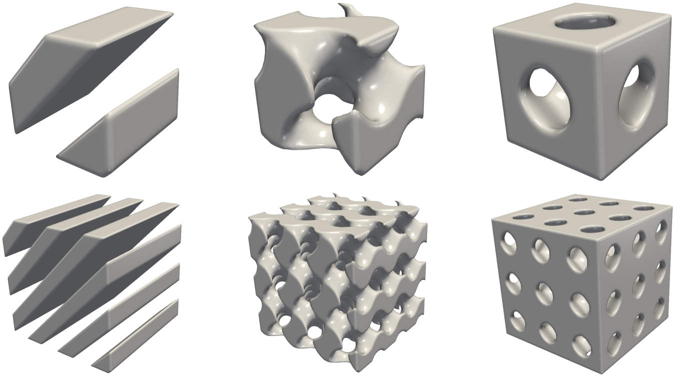
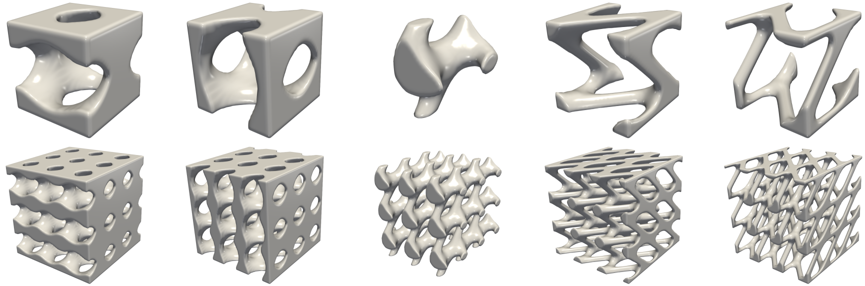
Influence of the perimeter penalty



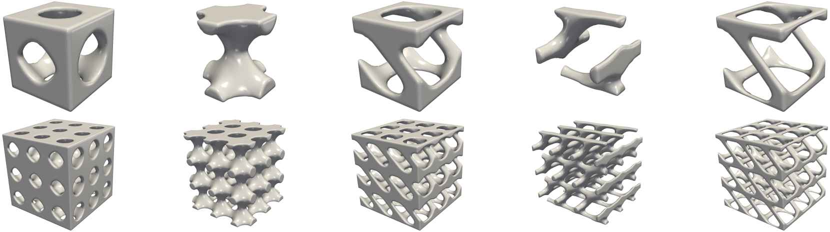
$\frac{1}{c_{Per}}$	2	4	10

Influence of relative Young's modulus



Load	B	P	B	P	B	P	B	P	B	P
1	0.063411	0.049912	0.096988	0.058266	0.1039	0.067704	0.10264	0.080092	0.10773	0.091178
2	0.03103	0.028423	0.043565	0.036762	0.032102	0.052916	0.024592	0.070516	0.026306	0.083817
3	0.031044	0.028416	0.044754	0.036902	0.032021	0.052907	0.024592	0.070516	0.026306	0.083817
4	0.039041	0.041364	0.048936	0.054934	0.064294	0.077477	0.080385	0.10026	0.092991	0.11802
5	0.039046	0.041362	0.048983	0.055215	0.064298	0.077457	0.080385	0.10026	0.092991	0.11802
6	0.012109	0.017901	0.012961	0.027966	0.010188	0.051458	0.005915	0.081734	0.0036466	0.10502
vol	0.41917	0.58083	0.3454	0.6546	0.25082	0.74918	0.16297	0.83703	0.10518	0.89482

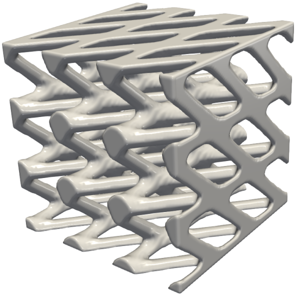
Influence of relative Young's modulus (cont.)



Load	B	P	B	P	B	P	B	P	B	P
1	0.036587	0.033904	0.047996	0.042686	0.06413	0.059585	0.06837	0.071062	0.088662	0.086567
2	0.049667	0.043946	0.070545	0.054043	0.076653	0.067548	0.072202	0.074892	0.093866	0.090007
3	0.035702	0.034632	0.050673	0.046461	0.023783	0.059513	0.039501	0.076961	0.02562	0.084978
4	0.032681	0.040275	0.033935	0.054312	0.027089	0.081685	0.0067487	0.090034	0.012522	0.11784
5	0.022299	0.031636	0.023708	0.046865	0.01006	0.065492	0.011444	0.094359	0.0046034	0.10924
6	0.035124	0.041468	0.04283	0.058455	0.060737	0.081456	0.097432	0.10662	0.088804	0.11808
vol	0.41037	0.58963	0.32744	0.67256	0.22565	0.77435	0.15367	0.84633	0.10194	0.89806

Physical case

Young's modulus of bone and polymer differ by a factor 15 and the Poisson ratios are given by $\nu^{\mathrm{b}} = 0.1$ and $\nu^{\mathrm{p}} = 0.3$. Further, we assume 1 compressions and 2 shears.



Outlook

- Full optimization of an entire scaffold under physiological loading conditions.
- Optimization for regeneration properties.
- Some analysis questions, e.g. regarding symmetry.

Thank you for your attention.