Supplementary

Appendix 1 Updating $\mathcal{Z}_l$

Noting that each group is independent, and removing the irrelevant terms, we have

$$\min_{\mathcal{Z}_l} \frac{1}{2}\left\| \mathcal{E}_l \mathcal{X}^{(k)} - \mathcal{Z}_l \times_1 \boldsymbol{D}_1^{(k)} \times_2 \boldsymbol{D}_2^{(k)} \right\|_F^2 + \frac{\rho}{4}\left\| \mathcal{B}_l^{(k)} - \mathcal{Z}_l - \mathcal{T}_l^{(k)} \right\|_F^2 \quad s.t. \ \left\| \mathcal{Z}_l \right\|_0 \le q_l \tag{1.1}$$

Defining $\boldsymbol{D}^{(k)} = \boldsymbol{D}_1^{(k)} \otimes \boldsymbol{D}_2^{(k)}$ with the symbol "$\otimes$" as Kronecker product of matrices, then [1.1] can be updated by

$$\min_{\boldsymbol{Z}_l} \frac{1}{2}\left\| \mathcal{E}_l \boldsymbol{X}_{(3)}^{(k)} - \boldsymbol{Z}_{l_{(3)}} \boldsymbol{D}^{(k)} \right\|_F^2 + \frac{\rho}{4}\left\| \boldsymbol{B}_{l_{(3)}}^{(k)} - \boldsymbol{Z}_{l_{(3)}} - \boldsymbol{T}_{l_{(3)}}^{(k)} \right\|_F^2 \tag{1.2}$$

where $\mathcal{E}_l \mathcal{X}^{(k)}, \mathcal{Z}_l, \mathcal{B}_l^{(k)}$ and $\mathcal{T}_l^{(k)}$ are unfolding the $\mathcal{E}_l \mathcal{X}^{(k)}, \mathcal{Z}_l, \mathcal{B}_l^{(k)}$ and $\mathcal{T}_l^{(k)}$ in the 3rd mode. To determine the minimal point of Eq. [1.2], the derivative of Eq. [1.2] should equal to zero. We have

$$\left(\boldsymbol{D}^{(k)}\right)^T \left(\boldsymbol{Z}_{l_{(3)}} \boldsymbol{D}^{(k)} - \mathcal{E}_l \boldsymbol{X}_{(3)}^{(k)} \right) + \frac{\rho}{2}\left(\boldsymbol{Z}_{l_{(3)}} - \boldsymbol{B}_{l_{(3)}}^{(k)} + \boldsymbol{T}_{l_{(3)}}^{(k)} \right) = 0 \tag{1.3}$$

Therefore, the $\boldsymbol{Z}_{l_{(3)}}$ can be updated by

$$\boldsymbol{Z}_{l_{(3)}}^{(k+1)} = \left(\left(\boldsymbol{D}^{(k)}\right)^T \left(\mathcal{E}_l \boldsymbol{X}_{(3)}^{(k)} \right) + \frac{\rho}{2}\left(\boldsymbol{B}_{l_{(3)}}^{(k)} - \boldsymbol{T}_{l_{(3)}}^{(k)} \right) \right) \left(\left(\boldsymbol{D}^{(k)}\right)^T \boldsymbol{D}^{(k)} + \frac{\rho}{2}\boldsymbol{I} \right)^{-1} \tag{1.4}$$

where $\boldsymbol{I}$ is an identity matrix. The tensor $\mathcal{Z}_l^{(k+1)}$ can be obtained by folding $\mathcal{V}$ at the 3rd mode.

Appendix 2 Updating $\mathcal{V}$

After substituting Eq. [7] into Eq. [9] and removing irrelevant terms, we have

$$\mathcal{V}^{(k+1)} = \arg\min_{\mathcal{V}} \left\{ \begin{array}{l} \frac{\kappa}{2}\sum_{s=1}^{S} w_s \sum_{i_2=2}^{I_2}\sum_{i_1=2}^{I_1} \left(\left| \mathcal{V}_{i_1,i_2,s} - \mathcal{V}_{(i_1-1),i_2,s} \right| + \left| \mathcal{V}_{i_1,i_2,s} - \mathcal{V}_{i_1,(i_2-1),s} \right| \right) \\ + \frac{\kappa_1}{2}\left\| \mathcal{X}^{(k+1)} - \mathcal{V} - \mathcal{W}^{(k)} \right\|_F^2 \end{array} \right\} \tag{2.1}$$

Assuming the amplitude of boundary gradient are zero, Eq. [2.1] can be further evolved into

$$\mathcal{V}^{(k+1)} = \arg\min_{\{\boldsymbol{V}_s\}_{s=1}^{S}} \sum_{s=1}^{S} \left(\frac{\kappa \times w_s}{2}\left(\left\| \partial_{i_1} \boldsymbol{V}_s \right\|_1 + \left\| \partial_{i_2} \boldsymbol{V}_s \right\|_1 \right) + \frac{\kappa_1}{2}\left\| \boldsymbol{X}_s^{(k+1)} - \boldsymbol{V}_s - \boldsymbol{W}_s^{(k)} \right\|_F^2 \right) \tag{2.2}$$

where $\partial_{i_1} \boldsymbol{V}_s = \mathcal{V}_{i_1,i_2,s} - \mathcal{V}_{(i_1-1),i_2,s}$ and $\partial_{i_2} \boldsymbol{V}_s = \mathcal{V}_{i_1,i_2,s} - \mathcal{V}_{i_1,(i_2-1),s}$. To obtain the optimized solution of [2.2], it can be converted into

$$\boldsymbol{V}_s^{(k+1)} = \arg\min_{\boldsymbol{v}_s} \left(\left\| \partial_{i_1} \boldsymbol{V}_s \right\|_1 + \left\| \partial_{i_2} \boldsymbol{V}_s \right\|_1 + \frac{\kappa_1}{(\kappa \times w_s)}\left\| \boldsymbol{X}_s^{(k+1)} - \boldsymbol{V}_s - \boldsymbol{W}_s^{(k)} \right\|_F^2 \right) \tag{2.3}$$

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Then, two variables $\boldsymbol{F}_{1s}$ and $\partial_{i_1}\boldsymbol{V}_s$ are introduced to replace $\partial_{i_1}\boldsymbol{V}_s$ and s^{th}. As for the s^{th} energy bin, Eq. [2.3] equals to

$$\underset{\boldsymbol{v}_s,\boldsymbol{F}_{1s},\boldsymbol{F}_{2s},\boldsymbol{E}_{1s},\boldsymbol{E}_{2s}}{\arg\min} = \left\{ \begin{array}{l} \left(\left\|\boldsymbol{F}_{1s}\right\|_1 + \left\|\boldsymbol{F}_{2s}\right\|_1\right) + \dfrac{2\kappa_1}{2\left(\kappa \times w_s\right)}\left\|\boldsymbol{X}_s^{(k+1)} - \boldsymbol{V}_s - \boldsymbol{W}_s^{(k)}\right\|_F^2 \\ + \dfrac{\kappa_2}{2}\left\|\boldsymbol{F}_{1s} - \partial_{i_1}\boldsymbol{V}_s - \boldsymbol{E}_{1s}\right\|_F^2 + \dfrac{\kappa_2}{2}\left\|\boldsymbol{F}_{2s} - \partial_{i_2}\boldsymbol{V}_s - \boldsymbol{E}_{2s}\right\|_F^2 \end{array} \right\} \quad [2.4]$$

where $\kappa_2 > 0$ is a coupling factor, and $\boldsymbol{E}_{1s}$ and $\boldsymbol{E}_{2s}$ represent the feedback errors. The objective function Eq. [2.4] can be divided into the following five sub-problems

$$\boldsymbol{V}_s^{(k+1)} = \underset{\boldsymbol{v}_s}{\arg\min}\left(\frac{\eta_s}{2}\left\|\boldsymbol{X}_s^{(k+1)} - \boldsymbol{V}_s - \boldsymbol{W}_s^{(k)}\right\|_F^2 + \left\|\boldsymbol{F}_{1s}^{(k)} - \partial_{i_1}\boldsymbol{V}_s - \boldsymbol{E}_{1s}^{(k)}\right\|_F^2 + \left\|\boldsymbol{F}_{2s}^{(k)} - \partial_{i_2}\boldsymbol{V}_s - \boldsymbol{E}_{2s}^{(k)}\right\|_F^2\right) \quad [2.5]$$

$$\boldsymbol{F}_{1s}^{(k+1)} = \overset{[2.5]}{\underset{\boldsymbol{F}_{1s}}{\arg\min}}\left\|\boldsymbol{F}_{1s}\right\|_1 + \frac{\kappa_2}{2}\left\|\boldsymbol{F}_{1s} - \partial_{i_1}\left(\boldsymbol{V}_s^{(k+1)}\right) - \boldsymbol{E}_{1s}^{(k)}\right\|_F^2 \quad [2.6]$$

$$\boldsymbol{F}_{2s}^{(k+1)} = \underset{\boldsymbol{F}_{2s}}{\arg\min}\left\|\boldsymbol{F}_{2s}\right\|_1 + \frac{\kappa_2}{2}\left\|\boldsymbol{F}_{2s} - \partial_{i_2}\left(\boldsymbol{V}_s^{(k+1)}\right) - \boldsymbol{E}_{2s}^{(k)}\right\|_F^2 \quad [2.7]$$

$$\boldsymbol{E}_{1s}^{(k+1)} = \boldsymbol{E}_{1s}^{(k)} - \left(\boldsymbol{F}_{1s}^{(k+1)} - \partial_{i_1}\left(\boldsymbol{V}_s^{(k+1)}\right)\right) \quad [2.8]$$

$$\boldsymbol{E}_{2s}^{(k+1)} = \boldsymbol{E}_{2s}^{(k)} - \left(\boldsymbol{F}_{2s}^{(k+1)} - \partial_{i_2}\left(\boldsymbol{V}_s^{(k+1)}\right)\right) \quad [2.9]$$

For $\eta_s = \frac{4\kappa_1}{\kappa \times w_s \times \kappa_2}$ in Eq. [2.5], different energy bins of multi-energy computed tomography (CT) images correspond to different values, which can be a limitation in practice. Thus, an adaptive weighting strategy is proposed and given as

$$\eta_s = \left(\frac{\sqrt{\left\|\boldsymbol{X}_s^{(k+1)} - \boldsymbol{V}_s^{(k)} - \boldsymbol{W}_s^{(k)}\right\|_F^2}}{\sqrt{\sum_{s=1}^{S}\left\|\boldsymbol{X}_s^{(k+1)} - \boldsymbol{V}_s^{(k)} - \boldsymbol{W}_s^{(k)}\right\|_F^2}}\right)^{-1}\eta \quad [2.10]$$

where η is an empirical parameter. Using Eq. [2.10] we can obtain weighted factor w_s by adaptively adjusted η_s for different energy bins. For Eq. [2.5], a Fourier transform based alternating minimization (51) is employed to obtain its solution, which can be given as

$$\begin{array}{l} \boldsymbol{V}_s^{(k+1)} = F_x^{-1}\left(F_{Num}/F_{Den}\right) \\ F_{Num} = \left(\hat{\partial}_{i_1}\right)^* \circ F_x\left(\boldsymbol{F}_{1s}^{(k)} - \boldsymbol{E}_{1s}^{(k)}\right) + \left(\partial_{i_2}\right)^* \circ F_x\left(\boldsymbol{F}_{2s}^{(k)} - \boldsymbol{E}_{2s}^{(k)}\right) + \eta_s\left(\hat{\boldsymbol{I}}\right)^* \circ F_x\left(\boldsymbol{X}_s^{(k+1)} - \boldsymbol{W}_s^{(k)}\right) \\ F_{Den} = \left(\hat{\partial}_{i_1}\right)^* \circ \left(\partial_{i_1}\right) + \left(\partial_{i_2}\right)^* \circ \left(\partial_{i_2}\right) + \eta_{sx}\left(\hat{\boldsymbol{I}}\right)^* \circ \left(\boldsymbol{I}\right) \end{array} \quad [2.11]$$

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where F_x represents Fourier transform, $\hat{\partial}_{i_1}$, $\hat{\partial}_{i_2}$ and $\hat{\boldsymbol{I}}$ represent the Fourier transform of operators, "$\complement$" denotes complex conjugacy and "$\circ$" defines component-wise multiplication, and the division is component-wise as well. As for Eq. [2.6] and Eq. [2.7], they have closed-form solutions in terms of soft-thresholding filtering:

$$\boldsymbol{F}_{1s}^{(k+1)} = \mathrm{soft}_{\frac{1}{\kappa_2}}\left(\partial_{i_1}\left(\boldsymbol{V}_s^{(k+1)}\right) - \boldsymbol{E}_{1s}^{(k)}\right) \quad [2.12]$$

$$\boldsymbol{F}_{2s}^{(k+1)} = \mathrm{soft}_{\frac{1}{\kappa_2}}\left(\partial_{i_2}\left(\boldsymbol{V}_s^{(k+1)}\right) - \boldsymbol{E}_{2s}^{(k)}\right) \quad [2.13]$$

References

51. Wang Y, Yang J, Yin W, Zhang Y. A new alternating minimization algorithm for total variation image reconstruction. SIAM Journal on Imaging Sciences 2008;1:248-72.

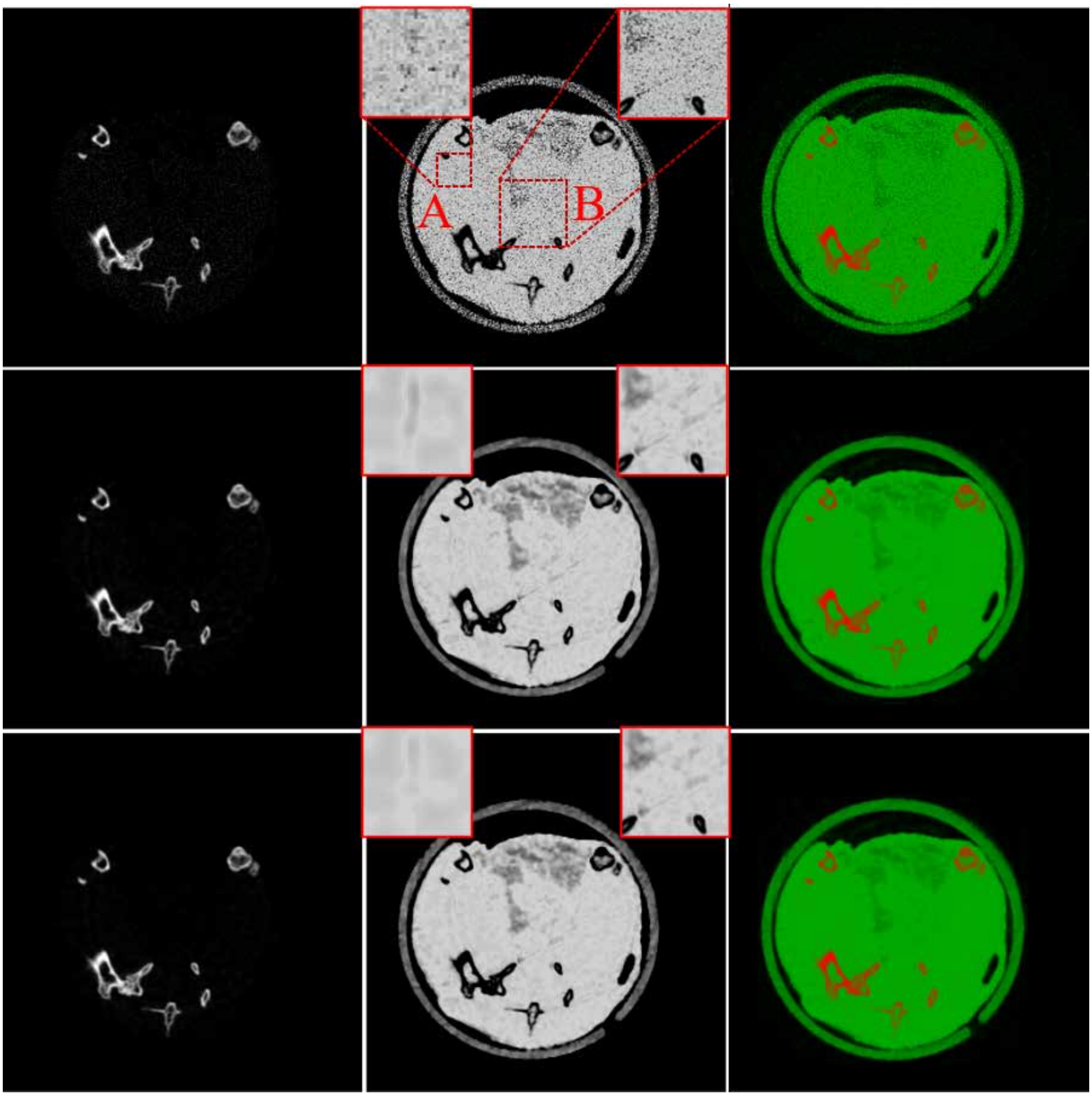

Figure S1 Materials decomposition results of preclinical mouse study. The 1st to 3rd columns are bone, soft tissue components, and color rendering. The corresponding display windows are [0 1] and [0.55 1.1]. A and B are two ROIs of the soft tissue component. ROIs, regions of interest.

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