Modeling and Simulation of magneto two-phase flow for magnetic drug targeting

TAG Mixtures Workshop 2025, Prague

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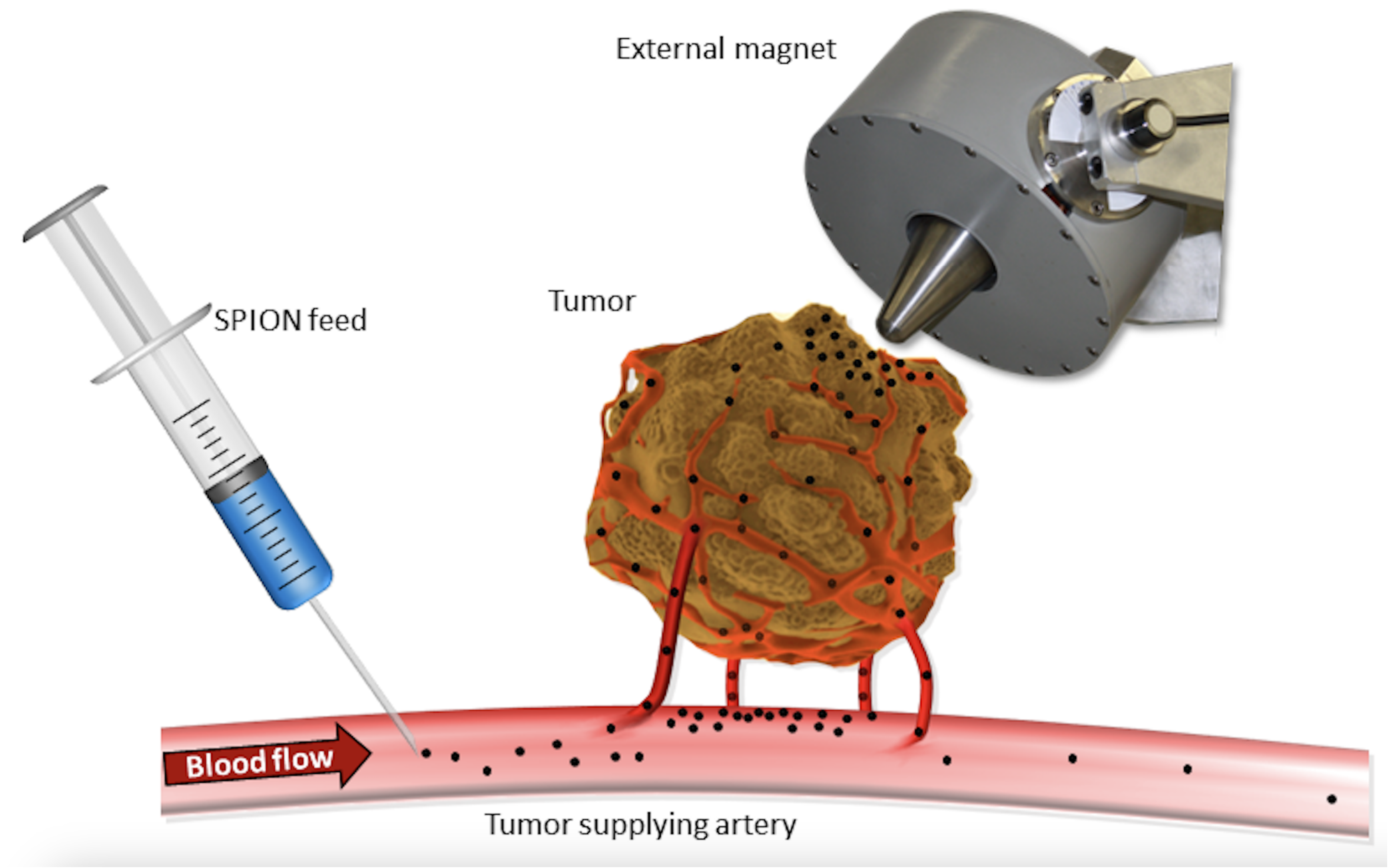
Motivation: Magnetic Drug Targeting

General Concept

- **DyNano**: **Dy**namics and Control of Superparamagnetic **Nano**particles in Simple and Branched Vessels



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  - Section for Experimental Oncology and Nanomedicine, University Hospital Erlangen
  - Chair for Technical Electronics, FAU Erlangen-Nürnberg
  - Chair for Applied Mathematics (Scientific Computing), FAU Erlangen-Nürnberg

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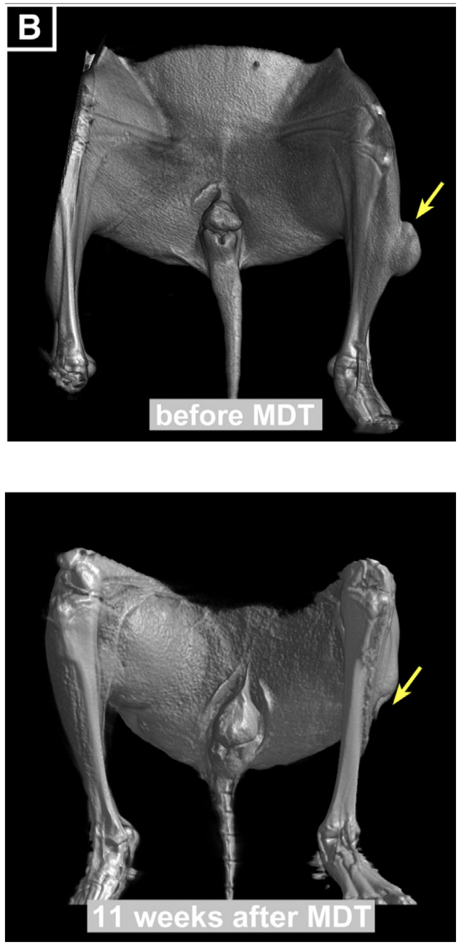

Modeling

Mass balance for two-phase flow

- Consider the **total mass density of a mixture**

$$\rho = \rho(t, x) := \rho_f(t, x) + \rho_p(t, x),$$

  with ρ_f, ρ_p: the current densities of the fluid and SPION particle phase
- The **mass balance** for individual phases reads

$$\partial_t \rho_j + \nabla \cdot (\rho_j \mathbf{v}_j) = 0, \qquad j \in \{f, p\},$$

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- Introducing the **volume density** of a phase

$$u_j(t,x) := \frac{1}{\widetilde{\rho}_j}\rho_j(t,x), \qquad \widetilde{\rho}_f, \widetilde{\rho}_p > 0,\ j \in \{f,p\},$$

and the **volume-averaged velocity of the mixture** **(Boyer 2002, Abels et al. 2012)**

$$\mathbf{v} := u_f \mathbf{v}_f + u_p \mathbf{v}_p,$$

we obtain the **modified mass balance equations**

$$\partial_t u_j + \nabla \cdot (u_j \mathbf{v} + u_j \mathbf{v}_{j,rel}) = 0, \qquad j \in \{f,p\}$$

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Mass and momentum balance for two-phase flow

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- Assume that we can describe the mixture as a single fluid with $\mathbf{v}$, which satisfies the following **law of momentum conservation** (Abels et al. 2012)

$$\rho \partial_t \mathbf{v} + ((\rho \mathbf{v} + \widetilde{\mathbf{J}}) \cdot \nabla) \mathbf{v} = \nabla \cdot \mathbf{T} - \nabla p + \mathbf{f},$$

  with the additional flux

$$\widetilde{\mathbf{J}} := \mathbf{J}_f + \mathbf{J}_p = (\tilde{\rho}_p - \tilde{\rho}_f) u_p \mathbf{v}_{p,rel},$$

  stress tensor $\mathbf{T}$, pressure p and force density $\mathbf{f}$.
- It remains to specify $\mathbf{T}$, $\mathbf{v}_{p,rel}$ and $\mathbf{f}$.

Modeling

The magnetic field

- We assume that the **magnetic field strength** $\mathbf{h}\colon (0,T) \times \Omega \to \mathbb{R}^n$ and the **magnetization** of the particles $\mathbf{m}\colon (0,T) \times \Omega \to \mathbb{R}^n$ are connected via the **magnetostatic equations with matter**, i.e.

$$\begin{aligned} \nabla \times \mathbf{h} &= 0, \\ \nabla \cdot (\mathbf{h} + \mathbf{m}) &= 0 \end{aligned}$$

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$$\nabla\cdot(\mathbf{h}+\mathbf{m})=0$$

- For $\mathbf{m}$, different choices are reasonable:

PDE for $\mathbf{m}$ **(Weiß et al. 2019)**

$$\frac{D'}{Dt}\mathbf{m}-\sigma\Delta\mathbf{m}=-\frac{1}{\tau_{rel}}(\mathbf{m}-\chi(u_p)\mathbf{h})$$

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$$\mathbf{m}=\chi(u_p)L(|\mathbf{h}|)\frac{\mathbf{h}}{|\mathbf{h}|}$$

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- With $\mathbf{h}=\nabla\phi$ we get a **quasi-static elliptic *Neumann* problem**

$$\nabla\cdot((1+\chi_0u_p)\nabla\phi)=0 \quad \text{in } (0,T)\times\Omega,$$
$$(1+\chi_0u_p)\nabla\phi\cdot\mathbf{n}=\mathbf{h}_e\cdot\mathbf{n} \quad \text{on } (0,T)\times\Omega,$$

with the external magnetic field $\mathbf{h}_e$.

Modeling

Constitutive relations

- We consider the following **energy and dissipation functionals**
  - **Potential energy**

$$\mathcal{E}_{\text{pot}}(t) := \int_\Omega \rho(u_p) g x_3 \mathrm{d}x$$

  - **Kinetic energy**

$$\mathcal{E}_{\text{kin}}(t) := \frac{1}{2}\int_\Omega \rho(u_p)|\mathbf{v}|^2 \mathrm{d}x$$

  - **Mixing energy**

$$\mathcal{E}_{\text{mix}}(t) := RT\int_\Omega \kappa_p u_p \ln\left(\frac{\kappa_p u_p}{\widetilde{c}_p}\right)\mathrm{d}x + RT\int_\Omega \kappa_f u_f \ln\left(\frac{\kappa_f u_f}{\widetilde{c}_f}\right)\mathrm{d}x$$

  - **Magnetic energy**

$$\mathcal{E}_{\text{mag}}(t) := \frac{\mu_0}{2}\int_\Omega \mathbf{h}\cdot(\mathbf{h}+\mathbf{m})\,\mathrm{d}x,$$

  - **Kinetic dissipation**

$$\mathcal{D}_{\text{kin}}(t) := \int_\Omega \frac{|\mathbf{T}|^2}{4\eta},$$

  - **Drag dissipation**

$$\mathcal{D}_{\text{drag}}(t) := \frac{N_A}{2}\int_\Omega \xi(u_p)|\mathbf{v}_{p,rel}|^2\,\mathrm{d}x,$$

where

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is a nonlinear friction coefficient

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Onsager's variational principle

$$\delta_{(\mathbf{T}, \mathbf{v}_{p,rel})} \Big(\mathcal{E}'_{\text{kin}}(t) + \mathcal{E}'_{\text{pot}}(t) + \mathcal{E}'_{\text{mix}}(t) + \mathcal{E}'_{\text{mag}}(t) + \mathcal{D}_{\text{kin}}(t) + \mathcal{D}_{\text{drag}}(t) \Big) = 0$$

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- Modified *Navier-Stokes* equation for the volume-averaged velocity $\mathbf{v}$ and the pressure p:

$$\rho(u_p)\partial_t \mathbf{v} + \left(\left(\rho(u_p)\mathbf{v} + \left(\frac{\widetilde{\rho}_p}{\widetilde{\rho}_f} - 1\right)\mathbf{v}_{p,rel}(u_p, \mathbf{h})\right) \cdot \nabla\right)\mathbf{v} - \frac{1}{Re}\Delta\mathbf{v} + \nabla p = \mathbf{f}(u_p, \mathbf{h}),$$

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- Transport equation for the SPION's volume density u_p:

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- Velocity $\mathbf{v}_{p,rel}$ of the SPIONs relative to the volume-averaged velocity $\mathbf{v}$ (with $\mathbf{h} = \nabla\phi$):

$$\mathbf{v}_{p,rel}(u_p,\mathbf{h}) := \underbrace{-\frac{1}{Pe}\kappa(u_p)\nabla u_p}_{\text{nonlinear diffusion}} \underbrace{- \frac{1}{Fr_*^2}u_p(1-u_p)\mathbf{e}_3}_{\text{drift due to gravity}} + \underbrace{\frac{1}{Ke_*^2}u_p(1-u_p)(\mathbf{h}\cdot\nabla)\mathbf{h}}_{\text{drift due to magnetic attraction}}$$

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- Elliptic equation for the magnetic potential ϕ:

$$\nabla \cdot \left((1 + \chi_0 u_p)\nabla\phi\right) = 0.$$

Discretization and implementation aspects

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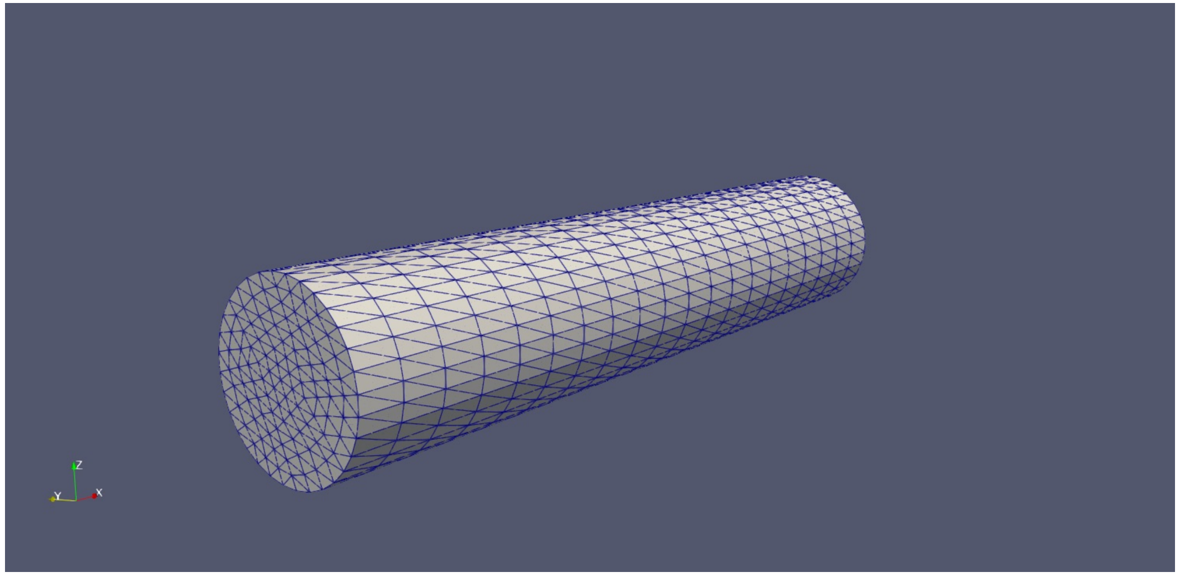

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4. Find $\mathbf{v}_h^0 \in \boldsymbol{\mathcal{V}}_{h,\Gamma_D}$ and $p_h^0 \in \mathcal{V}_h$ such that

$$\int_\Omega \left[\left(\rho(u_h^0) \mathbf{v}_h^0 + \left(\frac{\tilde{\rho}_p}{\tilde{\rho}_f} - 1 \right) \mathbf{v}_{p,rel}(u_h^0, \mathbf{h}_h^0) \right) \cdot \nabla \right] \mathbf{v}_h^0 \cdot \mathbf{w}_h \, \mathrm{d}x + \frac{1}{Re} \int \nabla \mathbf{v}_h^0 : \nabla \mathbf{w}_h \, \mathrm{d}x$$
$$+ \int_\Omega \mathbf{v}_0^h \cdot \nabla q_h \, \mathrm{d}x - \int_\Omega p_h^0 \nabla \cdot \mathbf{w}_h \, \mathrm{d}x = \int_\Omega \mathbf{f}(u_h^0, \mathbf{h}_h^0) \cdot \mathbf{w}_h \, \mathrm{d}x \qquad \forall (\mathbf{w}_h, q_h) \in \boldsymbol{\mathcal{V}}_{h,0} \times \mathcal{W}_h.$$

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3. Find $\mathbf{v}_h^n \in \boldsymbol{\mathcal{V}}_{h,\Gamma_D}$ and $p_h^n \in \mathcal{V}_h$ such that

$$\frac{1}{\tau} \int_\Omega \rho(u_h^{n-1}) \mathbf{v}_h^n \cdot \mathbf{w}_h \, \mathrm{d}x + \int_\Omega \left[\left(\rho(u_h^{n-1}) \mathbf{v}_h^n + \left(\frac{\tilde{\rho}_p}{\tilde{\rho}_f} - 1 \right) \mathbf{v}_{p,rel}(u_h^{n-1}, \mathbf{h}_h^n) \right) \cdot \nabla \right] \mathbf{v}_h^n \cdot \mathbf{w}_h \, \mathrm{d}x + \frac{1}{Re} \int \nabla \mathbf{v}_h^n : \nabla \mathbf{w}_h \, \mathrm{d}x$$
$$+ \int_\Omega \mathbf{v}_0^n \cdot \nabla q_h \, \mathrm{d}x - \int_\Omega p_h^n \nabla \cdot \mathbf{w}_h \, \mathrm{d}x = \int_\Omega \mathbf{f}(u_h^{n-1}, \mathbf{h}_h^n) \cdot \mathbf{w}_h \, \mathrm{d}x + \frac{1}{\tau} \int_\Omega \rho(u_h^{n-1}) \mathbf{v}_h^{n-1} \cdot \mathbf{w}_h \, \mathrm{d}x \quad \forall (\mathbf{w}_h, q_h) \in \boldsymbol{\mathcal{V}}_{h,0} \times \mathcal{W}_h.$$

For $n = 1, ..., N$ do:

1. Find $\phi_h^n \in \mathcal{V}_h$ such that

$$\int_\Omega (1 + \chi_0 u_h^{n-1}) \nabla \phi_h^n \cdot \nabla \psi_h \, \mathrm{d}x = - \int_{\partial\Omega} \mathbf{h}_e(t_n) \cdot \mathbf{n} \psi_h \mathrm{d}\sigma \quad \forall \psi_h \in \mathcal{V}_h.$$

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4. Find $u_h^n \in \mathcal{W}_h$ such that

$$\frac{1}{\tau} \int_\Omega u_h^n s_h \, \mathrm{d}x - \int_\Omega (\mathbf{v}_h^n u_h^n + \mathbf{v}_{p,rel}(u_h^n, \mathbf{h}_h^n)) \cdot \nabla s_h \, \mathrm{d}x =$$
$$\frac{1}{\tau} \int_\Omega u_h^{n-1} s_h \, \mathrm{d}x - \int_{\Gamma_{in}} u^{\text{in}}(t_n) \mathbf{v}_h^n \cdot \mathbf{n} s_h \mathrm{d}\sigma - \int_{\Gamma_{out}} u_h^n \mathbf{v}_{eff}(u_h^n, \mathbf{h}_h^n) \cdot \mathbf{n} s_h \mathrm{d}\sigma \qquad \forall s_h \in \mathcal{W}_h.$$

Simulation results

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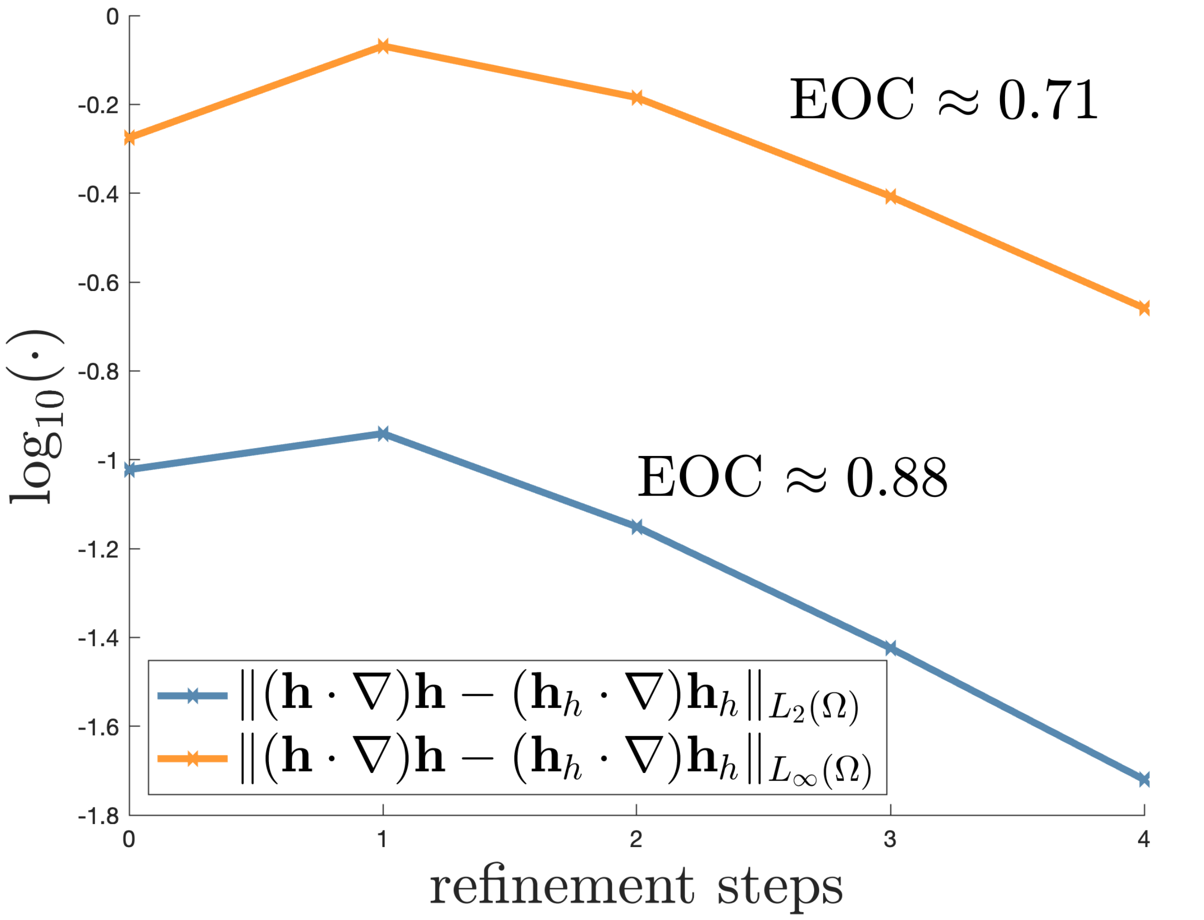

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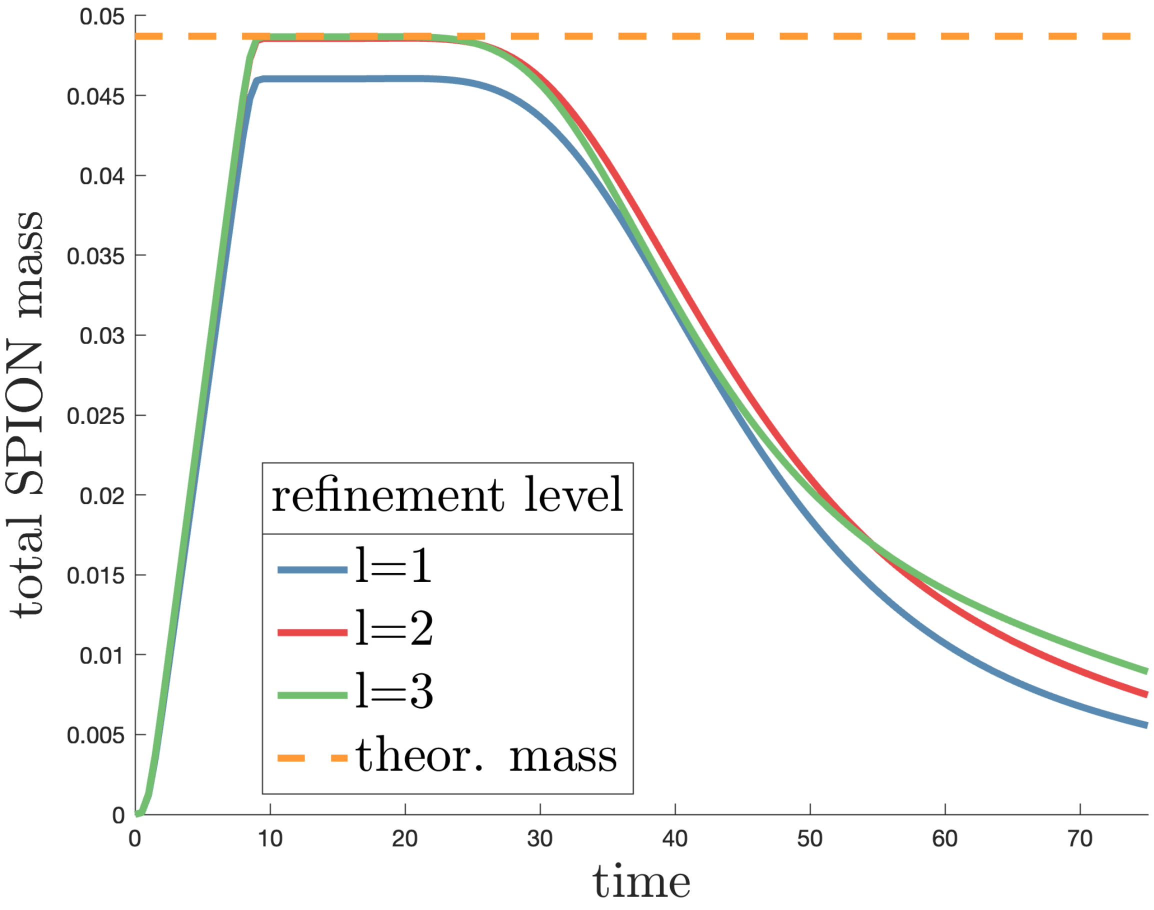
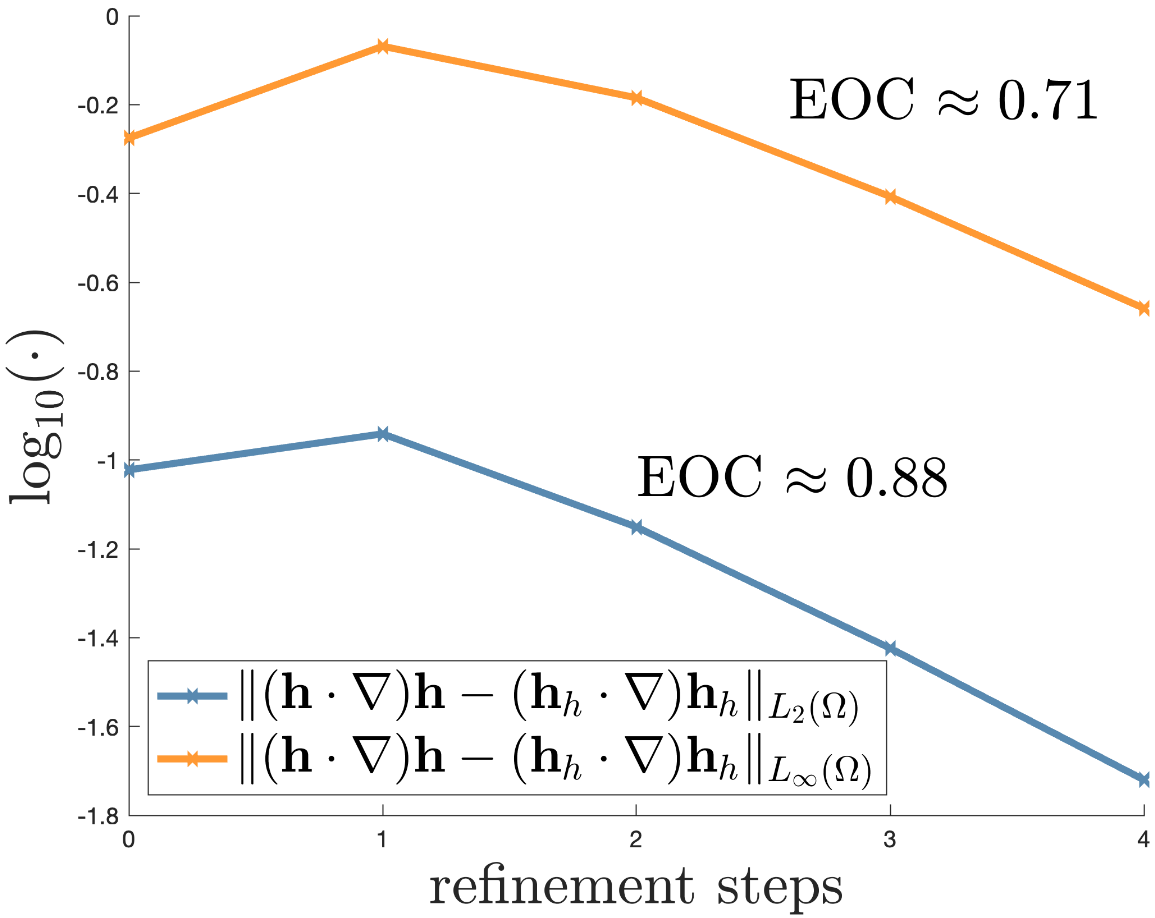
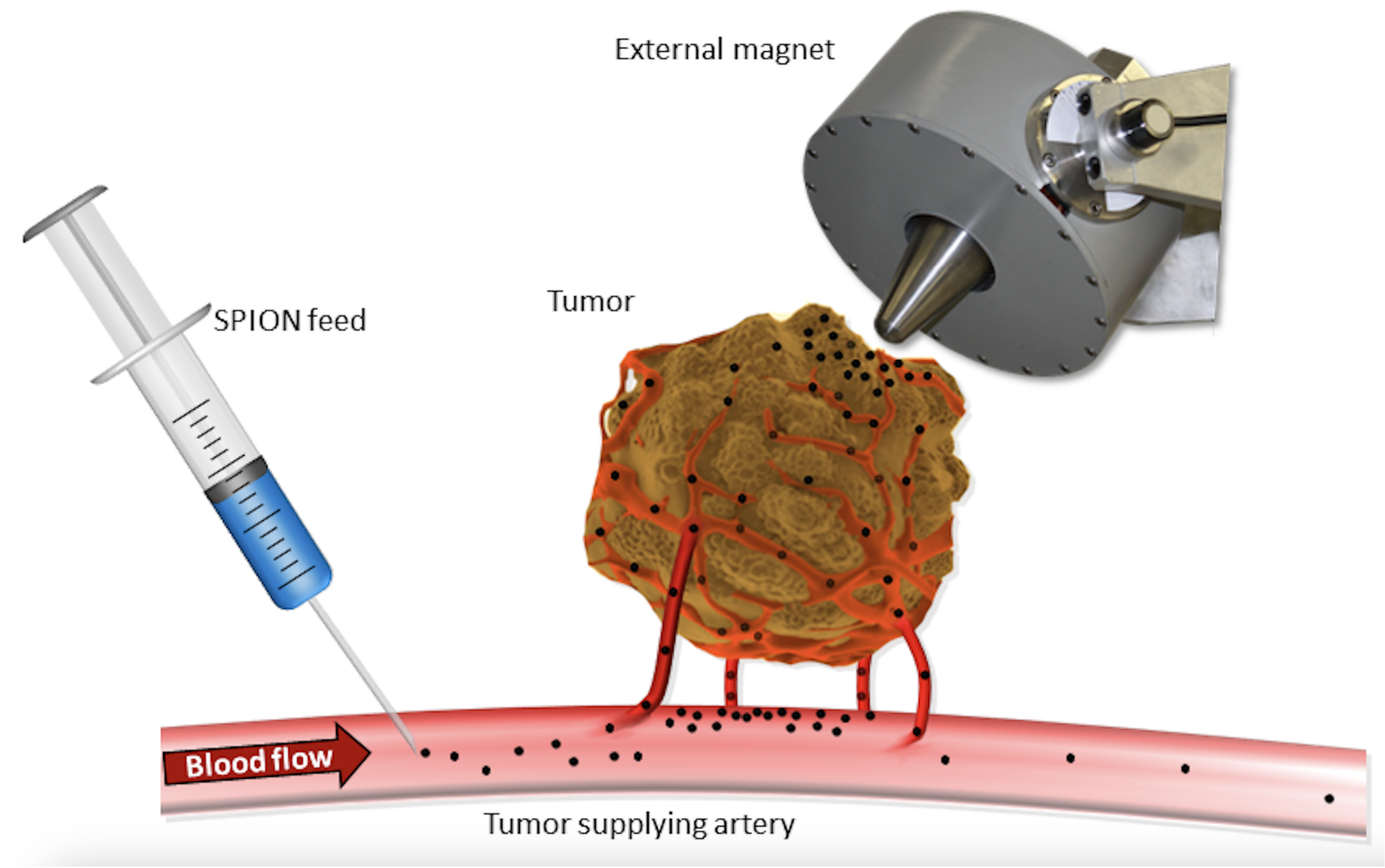




Outlook



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- Model transmission of particles into surrounding tissue
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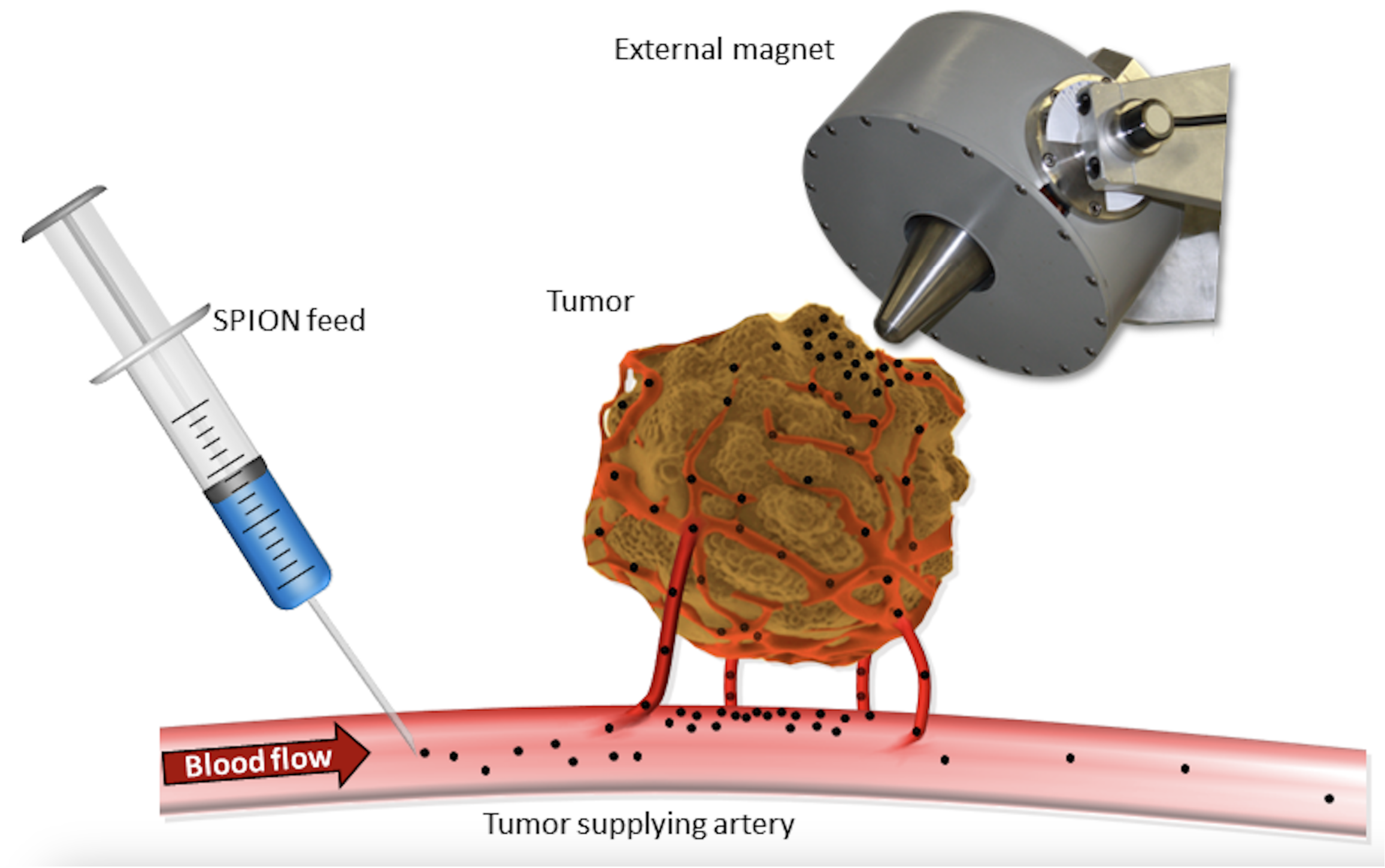

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Thank you for your attention!