Incorporating interface permeability into the Matrix Formalism representation of the diffusion MRI signal

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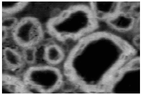
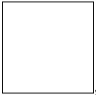
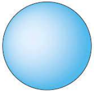
Why permeablility matters?

 $\Rightarrow$ ,  $\Rightarrow$ 

Traditional estimation model: Simple geometry + no water exchange between compartment $\Rightarrow$ Inaccurate.

E.x. Estimated volume fraction will be bigger than realistic value.

Khateri M., et al. (2022) *NMR Biomed*
What does FEXI measure?

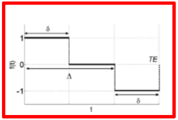
Objective

1. Generate fast diffusion MRI signal with different permeability values.
2. Propose a new reduced model, which helps permeability inference.

Bloch-Torrey equation

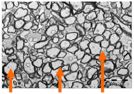
$$
\begin{aligned}
\frac{\partial}{\partial t} M^i(\boldsymbol{x}, t) &= \nabla \cdot (D^i \nabla M^i(\boldsymbol{x}, t)) - I\gamma f(t) \boldsymbol{g} \cdot \boldsymbol{x} M^i(\boldsymbol{x}, t), \boldsymbol{x} \in \Omega_i, && (1)\\
D^i \nabla M^i(\boldsymbol{x}, t) \cdot \boldsymbol{n}^i(\boldsymbol{x}) &= -D^j \nabla M^j(\boldsymbol{x}, t) \cdot \boldsymbol{n}^j(\boldsymbol{x}), \quad \boldsymbol{x} \in \Gamma_{ij}, && (2)\\
D^i \nabla M^i(\boldsymbol{x}, t) \cdot \boldsymbol{n}^i(\boldsymbol{x}) &= \kappa^{ij} (M^j(\boldsymbol{x}, t) - M^i(\boldsymbol{x}, t)), \quad \boldsymbol{x} \in \Gamma_{ij}, && (3)\\
M^i(\boldsymbol{x}, 0) &= \rho, \quad \boldsymbol{x} \in \Omega_i, && (4)\\
D^i \nabla M^i(\boldsymbol{x}, t) \cdot \boldsymbol{n}^i(\boldsymbol{x}) &= 0, \quad \boldsymbol{x} \in \partial\Sigma_i. && (5)
\end{aligned}
$$

$M^i(\boldsymbol{x}, t)$: Restriction of the complex transverse magnetization in Ω_i.
Conservation of water: $\kappa^{ij} = \kappa^{ji}$.



$$
f(t) = \begin{cases} 1, & 0 \le t \le \delta, \\ -1, & \Delta < t \le \Delta + \delta, \\ 0, & \text{otherwise}, \end{cases}
$$

Pulsed-gradient spin echo (PGSE)



$\Omega^i,\ D^i\ \kappa^{ie} \quad \Omega^e,\ D^e$

N_{cmpt} compartments: $N_{cmpt} - 1$ axons and one Extracellular space(ECS);
D: Diffusion coefficient;
ρ: initial spin.

Bloch-Torrey equation

dMRI signal

$$S(\delta,\Delta,\boldsymbol{g};\kappa) = \int_{\boldsymbol{x}\in\bigcup\Omega_i} M(\boldsymbol{x},T_E)\,d\boldsymbol{x} \tag{6}$$

- $\delta \nearrow$, $S(\delta,\Delta,\boldsymbol{g}) \searrow$;
- $\Delta \nearrow$, $S(\delta,\Delta,\boldsymbol{g}) \searrow$;
- $\|\boldsymbol{g}\| \nearrow$, $S(\delta,\Delta,\boldsymbol{g}) \searrow$;
- $\kappa \nearrow$, $S(\delta,\Delta,\boldsymbol{g}) \searrow$;
- Micro-structure estimation: Relate sequences parameters (δ,Δ and $\boldsymbol{g}$) to morphological parameters of interest.

A complete MRI experiment contains multiples sequences with different diffusion time, gradient strength and gradient directions.

Matrix Formalism representation

Idea: Decompose magnetization into a basis.

Theorem (Completeness of bounded Laplace operator)

Laplace operator in a bounded domain with Dirichlet,Neumann or Robin boundary condition has a complete set of eigenfunctions.

Laplace eigenmode

$$
\begin{aligned}
-\nabla \cdot D_i \nabla \phi_k^i(\boldsymbol{x}) &= \lambda_k \phi_k^i(\boldsymbol{x}), & \boldsymbol{x} \in \Omega_i, \quad (7)\\
D_i \nabla \phi_k^i(\boldsymbol{x}) \cdot \boldsymbol{n}^i(\boldsymbol{x}) &= -D_j \nabla \phi_k^j(\boldsymbol{x}) \cdot \boldsymbol{n}^j(\boldsymbol{x}), & \boldsymbol{x} \in \Gamma_{ij}, \quad (8)\\
D_i \nabla \phi_k^i(\boldsymbol{x}) \cdot \boldsymbol{n}^i(\boldsymbol{x}) &= \kappa_{ij}(\phi_k^j(\boldsymbol{x}) - \phi_k^i(\boldsymbol{x})), & \boldsymbol{x} \in \Gamma_{ij}, \quad (9)\\
D_i \nabla \phi_k^i(\boldsymbol{x}) \cdot \boldsymbol{n}^i(\boldsymbol{x}) &= 0, & \boldsymbol{x} \in \Sigma_i. \quad (10)
\end{aligned}
$$

- $(\lambda_k, \phi_k(\boldsymbol{x}))$: k-th L^2-normalized Laplace eigenpair on Ω;
- Eigenbasis $\{\phi_k(\boldsymbol{x})\}_{k=1,2,...}$ orthogonal;
- $0 = \lambda_1 < \lambda_2 \leq ...$ when $\kappa \neq 0 m/s$, $0 = \lambda_1 = ... = \lambda_{N_{cmpt}} < \lambda_{N_{cmpt}+1} \leq ...$ when $\kappa = 0 m/s$;
- $\int_\Omega \phi_k(\boldsymbol{x}) d\boldsymbol{x} = 0$ expect for those corresponding to 0 eigenvalue.

Matrix Formalism representation

$\Rightarrow$ We can decompose Bloch-Torrey operator into Laplace eigenbasis.
Rapidly oscillating eigenmodes do not contribute significantly to diffusion physics.
Length scale $l(\lambda_k) := \pi\sqrt{D_{ave}/\lambda_k}$, where $D_{ave} = \sum_{i=1}^{N_{cmpt}} D_i|\Omega_i|/|\Omega|$. Relate to wavelength.

$$M(\boldsymbol{x}, t) \approx \sum_{k=1}^{N_{eig}} \nu_k(t)\phi_k(\boldsymbol{x}) = \Phi(\boldsymbol{x})T(t),$$

where $T(t) = [\nu_1(t), \ldots, \nu_{N_{eig}}(t)]^T$, and $\Phi(\boldsymbol{x}) = [\phi_1(\boldsymbol{x}), \ldots, \phi_{N_{eig}}(\boldsymbol{x})]$.

Define $L = diag\left([\lambda_1, \ldots, \lambda_{N_{eig}}]\right)$. Multiplying ϕ_k and integral over Ω,

$$\frac{d}{dt}T(t) = -G(\boldsymbol{g})T(t), \tag{11}$$

$$G(\boldsymbol{g}) = L + I\gamma W(\boldsymbol{g}),$$

$$[W(\boldsymbol{g})]_{kl} = \int_\Omega \boldsymbol{g}\cdot\boldsymbol{x}\phi_k(\boldsymbol{x})\phi_l(\boldsymbol{x})\,d\boldsymbol{x}, \; (k,l) \in [[1, N_{eig}]]^2.$$

Matrix Formalism representation

dMRI signal in Matrix Formalism representation using PGSE

$$S(\delta,\Delta,\mathbf{g};N_{eig},\kappa) = \int_\Omega M(\boldsymbol{x},T_E)\,d\boldsymbol{x} = \int_\Omega \Phi^T(\boldsymbol{x})\cdot T(T_E)\,d\boldsymbol{x} = \int_\Omega \Phi^T(\boldsymbol{x})\cdot H(\mathbf{g},f)\cdot T(0)\,\rho\,d\boldsymbol{x}, \tag{12}$$

where

$$H(\mathbf{g},f;\kappa) = e^{-\delta\overline{G(\mathbf{g})}}\cdot e^{-(\Delta-\delta)L}\cdot e^{-\delta G(\mathbf{g})},$$

$$T(0) = \int_\Omega \Phi(\boldsymbol{x})\,d\boldsymbol{x}.$$

Discretized form of Matrix Formalism representation

In SpinDoctor, two steps: Eigendecompostion + signal computation.
Discretized the domain with P1 basis functions $\{\varphi_p(\boldsymbol{x})\}_{p\in\{1,\ldots,N_{nodes}\}}$.
Laplace eigenfunctions can be expressed onto P1 basis.
Multiplying $\varphi_p(\boldsymbol{x})$ with Laplace equation and integrating over Ω,

Generalized matrix eigenvalue problem

Find $L \in \mathbb{R}^{N_{eig},N_{eig}}$ and $\Phi \in \mathbb{R}^{N_{node},N_{eig}}$ satisfying

$$(K+Q)\cdot\Phi = M\cdot\Phi\cdot L, \tag{13}$$

where M is the mass matrix, K is the stiffness matrix, Q is the interface matrix.
$M, K, Q \in \mathbb{R}^{N_{node},N_{node}}$.

Discretized form of Matrix Formalism representation

dMRI signal in discretized form of Matrix Formalism

$$S(\delta,\Delta,\mathbf{g};N_{eig},\kappa) = \left(\mathbf{1}^T_{N_{node},1}\cdot M\cdot\Phi\right)H(\mathbf{g},f)\left(\Phi^T\cdot M\cdot\mathbf{1}_{N_{node},1}\right)\rho = T(0)^T H(\mathbf{g},f)\,T(0)\rho, \tag{14}$$

where $T(0)=\Phi^T\cdot M\cdot\mathbf{1}_{N_{node},1} = [\sqrt{|\Omega_1|},\ldots,\sqrt{|\Omega_{N_{group}}|},0,\ldots 0]^T$. When $\kappa = 0\,m/s$, $N_{group} = N_{cmpt}$.

$$H(\mathbf{g},f;\kappa) = e^{-\delta\overline{G(\mathbf{g})}}\cdot e^{-(\Delta-\delta)L}\cdot e^{-\delta G(\mathbf{g})}.$$

$$G(\mathbf{g}) = L + I\gamma W(\mathbf{g})$$

$$[W(\mathbf{g})]_{kl} = \int_\Omega \mathbf{g}\cdot\boldsymbol{x}\phi_k(\boldsymbol{x})\phi_l(\boldsymbol{x})\,d\boldsymbol{x} = \phi_k^T J\phi_l,\ (k,l)\in[[1,N_{eig}]]^2,$$

where

$$[J]_{pq} = \int_\Omega \mathbf{g}\cdot\boldsymbol{x}\varphi_p(\boldsymbol{x})\varphi_q(\boldsymbol{x})\,d\boldsymbol{x},\ (p,q)\in[[1,N_{node}]]^2.$$

- Reduce eigenvalue problem size from $N_{node}\times N_{node}$ to $N_{eig}\times N_{eig}$;
- Need to re-compute L and Φ when κ changes.

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Permeable diffusion MRI signal computation using impermeable eigenmodes

Idea: Always decompose $M(\boldsymbol{x},t)$ onto the impermeable Laplace eigenfunctions, as unperturbed state. Consider permeability as a perturbation.

The idea similar to

Grebenkov, Denis S. (2008) *Concepts in Magnetic Resonance*
Laplacian Eigenfunctions in NMR. I. A Numerical Tool

for permeable (Robin) boundary conditions.

The impermeable matrix eigenvalue problem:

Find $L_{imp} \in \mathbb{R}^{N_{eig},N_{eig}}$ and $\Phi_{imp} \in \mathbb{R}^{N_{node},N_{eig}}$ satisfying the eigenvalue matrix problem

$$K \cdot \Phi_{imp} = M \cdot \Phi_{imp} \cdot L_{imp}. \tag{15}$$

Impermeable Laplace eigenmode

$$\begin{aligned} -\nabla \cdot D_i \nabla \phi_k^i(\boldsymbol{x}) &= \lambda_k \phi_k^i(\boldsymbol{x}), && \boldsymbol{x} \in \Omega_i, \\ D_i \nabla \phi_k^i(\boldsymbol{x}) \cdot \boldsymbol{n}^i(\boldsymbol{x}) &= 0, && \boldsymbol{x} \in \Gamma_{ij}, \\ D_i \nabla \phi_k^i(\boldsymbol{x}) \cdot \boldsymbol{n}^i(\boldsymbol{x}) &= 0, && \boldsymbol{x} \in \Sigma_i. \end{aligned}$$

Permeable diffusion MRI signal computation using impermeable eigenmodes

We define perturbation matrix $Q_p \in \mathbb{R}^{N_{eig},N_{eig}}$,

$$Q_p(\kappa) = \Phi_{imp}^T \cdot Q \cdot \Phi_{imp},$$

$$[Q_p]_{kl} = \int_{\bigcup_{ij}\Gamma_{ij}} \mathrm{sgn}_{ij}(k,l)\kappa_{ij}\phi_{imp,k}(\boldsymbol{x})\phi_{imp,l}(\boldsymbol{x})\,d\boldsymbol{x},\ (k,l) \in [[1, N_{eig}]]^2,$$

where

$$\mathrm{sgn}_{ij}(k,l) = \begin{cases} 1, \text{ if } \phi_{imp,k} \text{ and } \phi_{imp,l} \text{ localized in the same compartment,} \\ -1, else, \end{cases}$$

the integral over the interfaces of pair-wise impermeable Laplace eigenfunctions.

Permeable signal using impermeable eigenmodes

Theorem (dMRI signal using impermeable eigenmodes)

$$S_{new}(\delta,\Delta,\mathbf{g},\kappa;N_{eig}) = \left(\mathbf{1}^T_{N_{node},1}\cdot M\cdot\Phi_{imp}\right) H_{mod}(\mathbf{g},f)\left(\Phi^T_{imp}\cdot M\cdot\mathbf{1}_{N_{node},1}\right)\rho, \qquad (16)$$

$$H_{mod}(\mathbf{g},f,\kappa) = e^{-\delta\overline{(L_{imp}+Q_p(\kappa)+I\gamma W_{imp}(\mathbf{g}))}}\cdot e^{-(\Delta-\delta)(L_{imp}+Q_p(\kappa))}\cdot e^{-\delta(L_{imp}+Q_p(\kappa)+I\gamma W_{imp}(\mathbf{g}))}$$

Compare to original

$$S_{per}(\delta,\Delta,\mathbf{g};N_{eig},\kappa) = \left(\mathbf{1}^T_{N_{node},1}\cdot M\cdot\Phi\right) H(\mathbf{g},f)\left(\Phi^T\cdot M\cdot\mathbf{1}_{N_{node},1}\right)\rho. \qquad (17)$$

$$H(\mathbf{g},f;\kappa) = e^{-\delta\overline{(L+I\gamma W(\mathbf{g}))}}\cdot e^{-(\Delta-\delta)L}\cdot e^{-\delta(L+I\gamma W(\mathbf{g}))}.$$

Replacing original quantities with impermeable quantities

$$\Phi\to\Phi_{imp},$$

$$W(\mathbf{g})\to W_{imp}(\mathbf{g}),$$

$$L\to(L_{imp}+Q_p),\ Q_p=\Phi^T_{imp}\cdot Q\cdot\Phi_{imp}.$$

Sketch of proof

(1) Using full set. $N_{eig} = N_{node}$
Define $C \equiv \Phi_{imp}^T \cdot M \cdot \Phi$. $\Rightarrow$ C is a unitary matrix, $C \cdot C^T = Id$.
Two consequences immediate:

- $\Phi_{imp} = \Phi \cdot C^T$;
- $L_{imp} + Q_p = \Phi_{imp}^T (K+Q) \Phi_{imp} = C \cdot \Phi^T (K+Q) \Phi \cdot C^T = C \cdot L_{per} \cdot C^T$.

$$
\begin{aligned}
S_{new}(\delta, \Delta, \mathbf{g}, \kappa; N_{node}) &= \left(\mathbf{1}_{N_{node},1}^T \cdot M \cdot \Phi_{imp}\right) H_{mod}(\mathbf{g}, f, \kappa) \left(\Phi_{imp}^T \cdot M \cdot \mathbf{1}_{N_{node},1}\right) \rho \\
&= \mathbf{1}_{N_{node},1}^T \cdot M \cdot \left(\Phi_{imp} \cdot C\right) \cdot H_{per}(\mathbf{g}, f; \kappa) \cdot \left(C^T \cdot \Phi_{imp}^T\right) \cdot M \cdot \mathbf{1}_{N_{node},1} \rho \\
&= \left(\mathbf{1}_{N_{node},1}^T \cdot M \cdot \Phi\right) H_{per}(\mathbf{g}, f; \kappa) \left(\Phi^T \cdot M \cdot \mathbf{1}_{N_{node},1}\right) \rho \\
&= S_{per}(\delta, \Delta, \mathbf{g}; N_{node}, \kappa).
\end{aligned} \tag{18}
$$

New method and Matrix Formalism are equivalent when $N_{eig} = N_{node}$.
(2) $N_{eig} < N_{node}$
$L_{imp} + Q_p = V \cdot \Lambda \cdot V^T = (C + \epsilon_2)(L_{per} + \epsilon_1)(C + \epsilon_2)^T$, $\Phi_{imp} = \Phi_{per} \cdot C^T + \epsilon_3$
$\epsilon_1, \epsilon_2, \epsilon_3 \xrightarrow[N_{eig} \to N_{node}]{} 0$, but not monotonously.

Properties of new method

Advantages

- Compute eigendecomposition once;
- Impermeable Laplace eigenfunctions are localized in one compartment $\Rightarrow$ They can be computed separately.

Disadvantages

- Need more eigenmodes to reach the same error level compared to Matrix Formalism.

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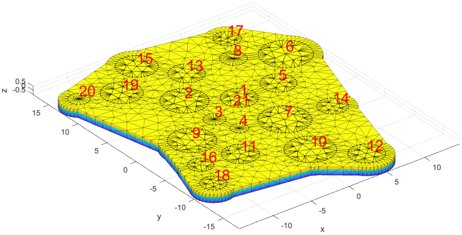
Experimental Setup

- 20 axons and 1 extracellular space(ECS), connecting through permeable interface;
- volume fraction of axons is 35.0%;
- Diffusion $\sigma = 2 \cdot 10^{-3}\, mm^2/s$;
- Permeability from $10^{-5}\, m/s$ to $10^{-4}\, m/s$, around $10^{-5}\, m/s$ for axonal membranes and myelin sheath depend on the temperature;
- 3 PGSE sequences, $\delta = \Delta$, hard case;
- Maximum g-value < 1T/m;
- Reference: Full set Matrix Formalism $S_{per}(\delta, \Delta, \mathbf{g}; N_{node}, \kappa)$;
- Criteria: Relative error < 1%.



Numerical validation: Full set

Direction averaged relative error (%) =
$100 \times 1/18 \sum_{d=1}^{18} |S_{per}(\delta, \Delta, \mathbf{g}_d; N_{node}, \kappa) - S_{new}(\delta, \Delta, \mathbf{g}_d, \kappa; N_{eig})| / S_{per}(\delta, \Delta, \mathbf{g}_d; N_{node}, \kappa)$,
where $\mathbf{g}_d = \|\mathbf{g}\| [cos(\pi \frac{d}{18}), sin(\pi \frac{d}{18}), 0]^T$.

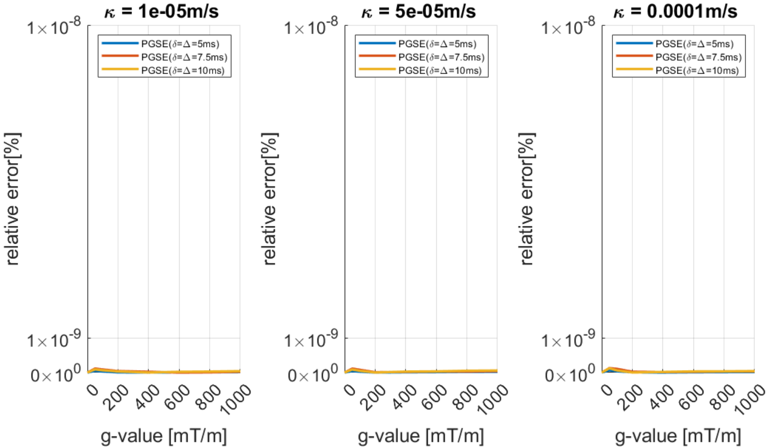


Figure: $N_{eig} = 3445$ (full set)

Numerical validation: $N_{eig} = 538$

- Proportional to diffusion time.

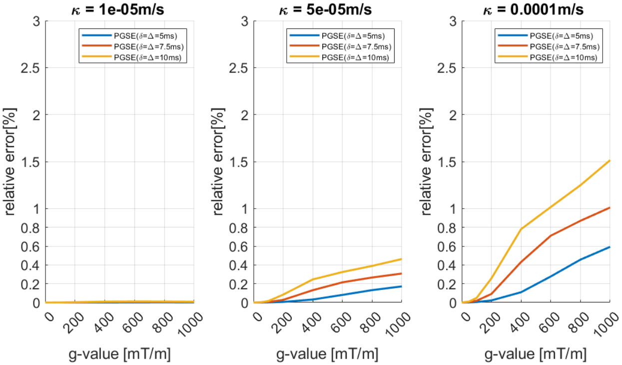


Figure: Length scale = 1 ($N_{eig} = 538$)

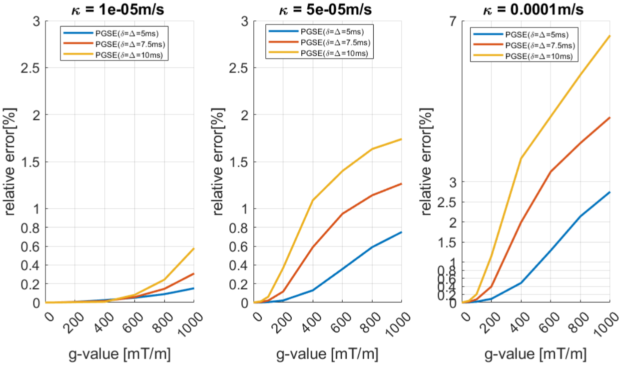
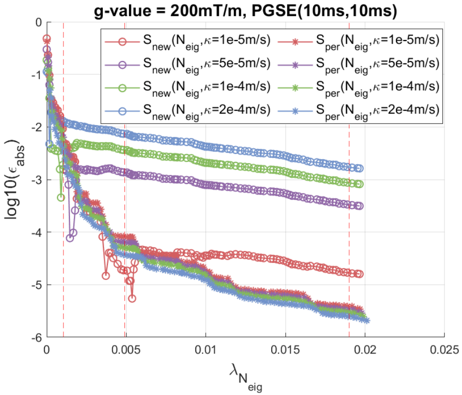
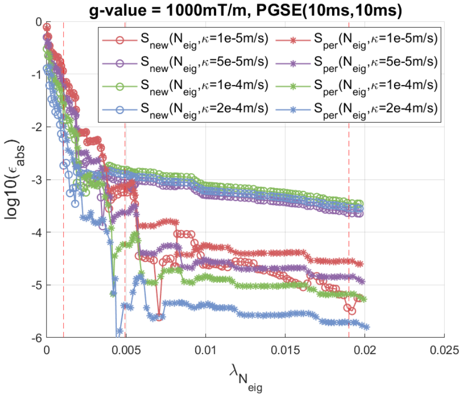
- 

Figure: Length scale = 2 ($N_{eig} = 193$)

Convergence rate

$\epsilon_{abs} = |S_{per}(\delta, \Delta, \mathbf{g}; N_{node}, \kappa) - S_i(\delta, \Delta, \mathbf{g}, \kappa; N_{eig})|/|\Omega|$, $i = \{new, per\}$.
Direction $[\sqrt{2}/2, \sqrt{2}/2, 0]^T$.





- The error deceases at the same rate for both methods in the beginning ($N_{eig} \leq 70$);
- When $N_{eig} > 70$, the error by new method deceases slower than Matrix Formalism;
- Require more eigenmodes to reach the same error level for new method.

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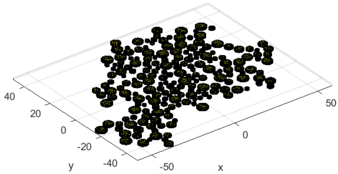
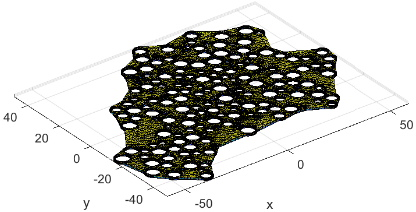
Computational time: eigen-decomposition





		Time(s)			
	$\kappa\,(m/s)$	$N_{eig} = 2000$	$N_{eig} = 4000$	$N_{eig} = 5000$	Full set
New method	0	41	171	278	141
Matrix Formalism	10^{-5}	99	419	646	723
	5×10^{-5}	100	389	518	727
	10^{-4}	102	353	625	734

Full set: 32023 nodes. ECS contains 16924 nodes.

Computational time: matrix exponential

$$\epsilon_{rel}(\%) = 100 \times \frac{|\bar{S}_{per}(\delta,\Delta,\mathbf{g}_{xy};N_{node},\kappa) - \bar{S}_{new}(\delta,\Delta,\mathbf{g}_{xy},\kappa;N_{eig})|}{\bar{S}_{per}(\delta,\Delta,\mathbf{g}_{xy};N_{node},\kappa)},$$

where $\mathbf{g}_{xy} = \|\mathbf{g}\|[\sqrt{2}/2, \sqrt{2}/2, 0]^T$.

When N_{eig} is the same, the time is the same. ⇒ Save eigen-decomposition time.

κ	δ	Δ	$\|\mathbf{g}\|$	Matrix Formalism + 100s		New method + 41s		FE
				Time	ϵ_{rel}	Time	ϵ_{rel}	Time
10^{-5}	5	5	200	1.2	0.0069	1.1	0.0023	34.0
			1000	1.8	0.27	2.3	0.066	117.3
	10	10	200	1.2	0.017	1.5	0.022	53.1
			1000	3.5	0.86	3.8	0.14	199.0
10^{-4}	5	5	200	1.2	0.0063	1.0	0.11	37.7
			1000	2.7	0.21	1.7	2.6	94.6
	10	10	200	1.7	0.014	1.2	1.3	56.6
			1000	4.7	0.39	3.7	6.1	179.9

Table: $N_{eig} = 2000$. δ and Δ in μs, $\|\mathbf{g}\|$ in mT/m, κ in m/s. Direction = $[\sqrt{2}/2, \sqrt{2}/2, 0]^T$.

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Signal contribution comparison

$T_{imp}(0) = [\sqrt{|\Omega_1|}, \ldots, \sqrt{\Omega_{N_{cmpt}}}, 0, \ldots, 0]^T \Rightarrow$ Only first $N_{cmpt} \times N_{cmpt}$ items of $H_{mod}(\mathbf{g}, f, \kappa)$ are needed in signal computation.
The volume-normalized signal as

$$\bar{S}_{new}(\delta, \Delta, \mathbf{g}, \kappa; N_{eig}) = \frac{S_{new}(\delta, \Delta, \mathbf{g}, \kappa; N_{eig})}{|\Omega|} = \sum_{i=1}^{N_{cmpt}} \sum_{j=1}^{N_{cmpt}} \sqrt{\frac{|\Omega_i|}{|\Omega|}} [H_{mod}(\mathbf{g}, f, \kappa)]_{ij} \sqrt{\frac{|\Omega_j|}{|\Omega|}}, \tag{19}$$

where
$H_{mod}(\mathbf{g}, f, \kappa) = e^{-\delta \overline{(L_{imp} + Q_p(\kappa) + I\gamma G_{imp}(\mathbf{g}))}} e^{-(\Delta-\delta)(L_{imp} + Q_p(\kappa))} e^{-\delta (L_{imp} + Q_p(\kappa) + I\gamma G_{imp}(\mathbf{g}))}$.
Define signal contribution as:

$$S_k(\delta, \Delta, \mathbf{g}, \kappa; N_{eig}) = \sum_{i=1}^{N_{cmpt}} \sum_{j=1}^{N_{cmpt}} \left(\sqrt{\frac{|\Omega_i|}{|\Omega|}} \bar{w}_{ki}\right) e^{-(\Delta-\delta)(L_{imp} + Q_p(\kappa))} \left(w_{kj} \sqrt{\frac{|\Omega_j|}{|\Omega|}}\right), \tag{20}$$

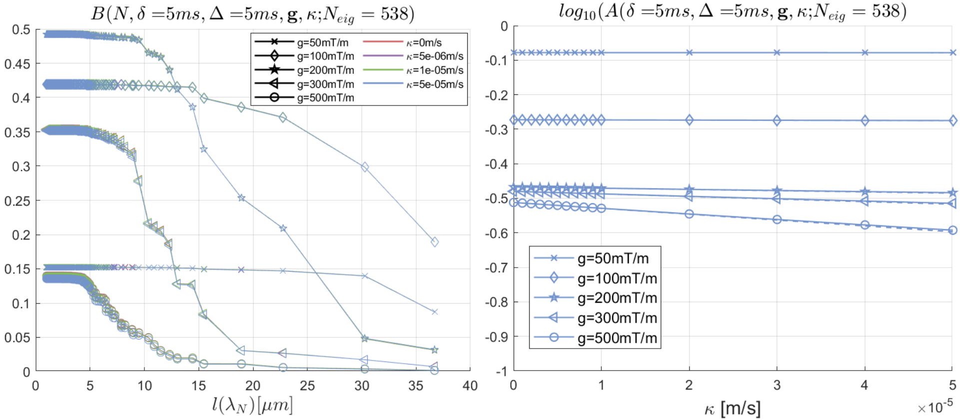
where w_{kj} is the k-th row, j-th column of the matrix $e^{-\delta (L_{imp} + Q_p(\kappa) + I\gamma G_{imp}(\mathbf{g}))}$.

$$\bar{S}_{new}(\delta, \Delta, \mathbf{g}, \kappa; N_{eig}) = \sum_{k=1}^{N_{eig}} S_k = \sum_{k=1}^{N_{cmpt}} S_k + \sum_{k=N_{cmpt}+1}^{N_{eig}} S_k = A(\delta, \Delta, \mathbf{g}, \kappa; N_{eig}) + \sum_{k=N_{cmpt}+1}^{N_{eig}} S_k.$$

Signal contribution comparison

Define $B(N, \delta, \Delta, \mathbf{g}, \kappa; N_{eig}) := \sum_{k=N_{cmpt}+1}^{N} S_k, N \in [[N_{cmpt}+1, N_{eig}]]$.

Simulated direction $[\sqrt{2}/2, \sqrt{2}/2, 0]^T$.



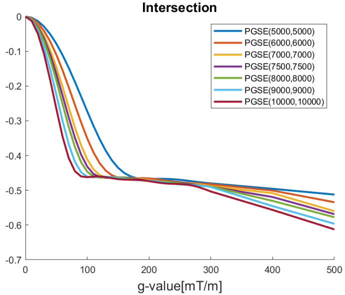
- $B(N, \delta, \Delta, \mathbf{g}, \kappa; N_{eig})$ is independent to κ in small permeability range;
- $A(\delta, \Delta, \mathbf{g}, \kappa; N_{eig})$ has an exponential relation with κ in small permeability range;
- $\bar{S}_{new}(\delta, \Delta, \mathbf{g}, \kappa; N_{eig}) = B(N_{eig}, \delta, \Delta, \mathbf{g}; N_{eig}) + A(\delta, \Delta, \mathbf{g}, \kappa; N_{eig})$.

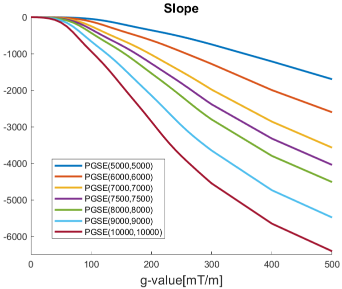
Approximation model for low permeable case

Reduced model for low permeability case

$$\bar{S}_{new}(\delta,\Delta,\mathbf{g},\kappa;N_{eig}) \approx \bar{S}_{imp}(\delta,\Delta,\mathbf{g};N_{eig}) + 10^{\alpha(\delta,\Delta,\mathbf{g})}(10^{\beta(\delta,\Delta,\mathbf{g})\cdot\kappa} - 1) = \bar{S}_{approx}, \quad (22)$$

where $\bar{S}_{imp}(\delta,\Delta,\mathbf{g};N_{eig})$ is the impermeable diffusion MRI signal,
$\bar{S}_{imp}(\delta,\Delta,\mathbf{g};N_{eig}) = B(N_{eig},\delta,\Delta,\mathbf{g};N_{eig}) + 10^{\alpha(\delta,\Delta,\mathbf{g})}$.
$\alpha(\delta,\Delta,\mathbf{g})$ and $\beta(\delta,\Delta,\mathbf{g})$ are intersection and slope of $log_{10}(A(\kappa))$, respectively.
$A(\delta,\Delta,\mathbf{g},\kappa;N_{eig}) = 10^{\beta(\delta,\Delta,\mathbf{g})\kappa+\alpha(\delta,\Delta,\mathbf{g})}$

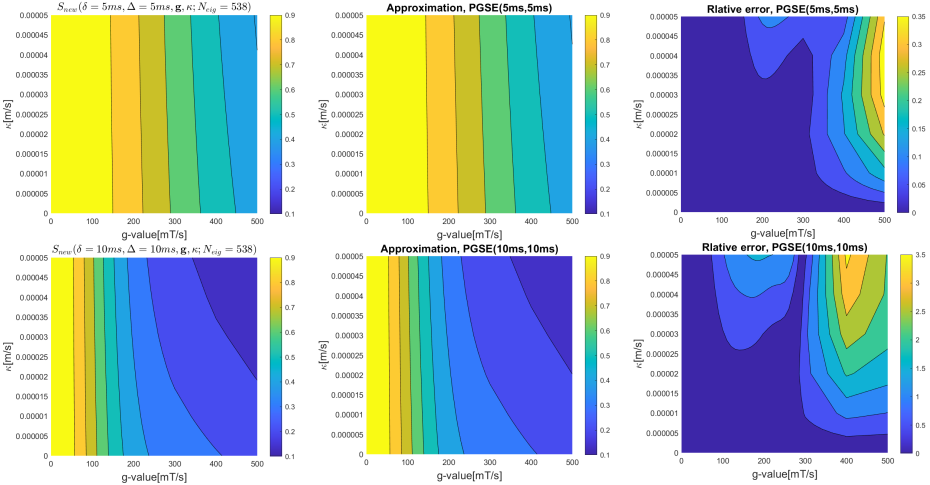




Hard to get simple relation between sequence and $\alpha(\delta,\Delta,\mathbf{g})$, $\beta(\delta,\Delta,\mathbf{g})$.

Simulation

$$\epsilon_{rel}(\%) = 100 \times \frac{|\bar{S}_{new}(\delta,\Delta,\mathbf{g},\kappa;N_{eig}) - \bar{S}_{approx}(\delta,\Delta,\mathbf{g},\kappa;N_{eig})|}{\bar{S}_{new}(\delta,\Delta,\mathbf{g},\kappa;N_{eig})}.$$



Modified approximation model for different geometries

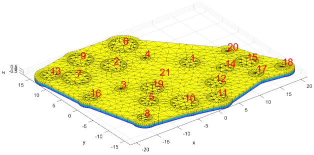


Figure: Geometry 2. Volume fraction = 25.7%.

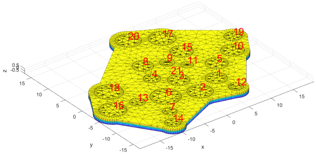


Figure: Geometry 3. Volume fraction = 32.3%.

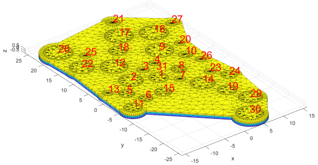


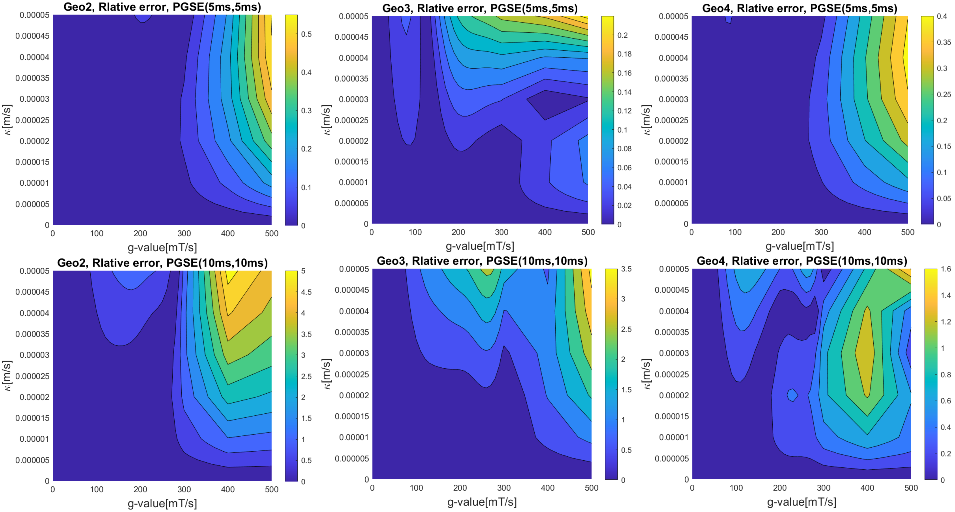
Figure: Geometry 4. Volume fraction = 31.2%.

Modified reduced model for different geometries

$$\bar{S}_{approx,geo_i} = \bar{S}_{imp,geo_i} + \frac{V_{f,geo_i}}{V_{f,geo_1}} 10^{\alpha_{geo_1}} (10^{\beta_{geo_1} \cdot \kappa} - 1), \quad (23)$$

where V_f is the volume fraction of axons. The subscript geo_i indicates the geometry i.

Simulation



Geo2, Rlative error, PGSE(5ms,5ms)
Geo3, Rlative error, PGSE(5ms,5ms)
Geo4, Rlative error, PGSE(5ms,5ms)
Geo2, Rlative error, PGSE(10ms,10ms)
Geo3, Rlative error, PGSE(10ms,10ms)
Geo4, Rlative error, PGSE(10ms,10ms)
κ[m/s]
g-value[mT/s]

Table of Contents

Outlook and future work

Outlook

- A new simulation to compute diffusion MRI signal with permeable interface, using Matrix Formalism representation with impermeable Laplace eigenfunctions;
- A new reduce model yielding approximate diffusion MRI signal in the case of low permeability.

Future work

- Permeability estimation;
- Morphological parameters estimation with permeable interface.

Thank you for your attention.