Stochastic Galerkin Method in Particle and Spin Tracking

Jamal Slim

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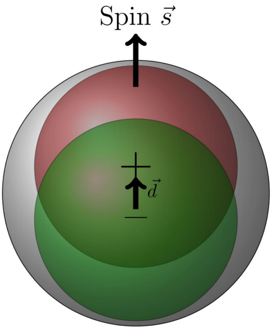
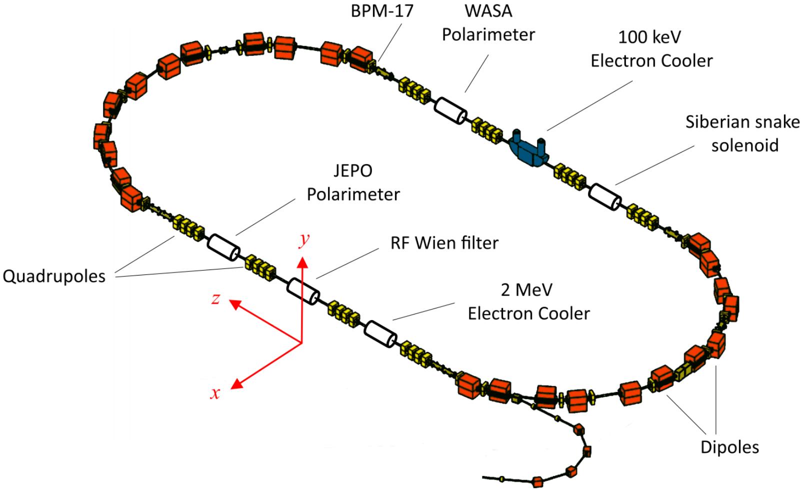
Motivation

- Permanent separation of positive and negative charge
- Fundamental property of particles
- Existence of EDM is only possible via violation of time reversal T and parity P symmetry
- Predominance of matter over antimatter in the Universe

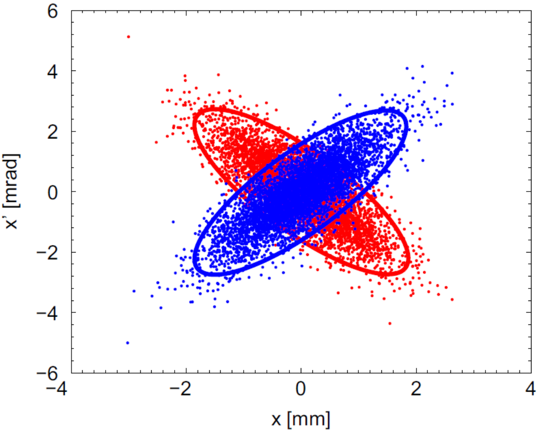


The Cooler Synchrotron (COSY)



The RF Wien filter: requirements

- An RF device that manipulates the polarization without inducing beam oscillations.
- Orthogonality between the electric and magnetic fields
- High-field homogeneity
- Vanishing Lorentz force



Polynomial Chaos Expansion (PCE)

The polynomial chaos expansion (PCE) is a stochastic spectral method that allows for stochastically varying physical entities $\mathcal{Y}$, as a response of some random input ξ to be represented in terms of orthogonal polynomials. PCE permits $\mathcal{Y}$ to be expanded into a series of orthogonal polynomials of degree p (the expansion order) as function of the input variables ξ.

$$\mathcal{Y} = \sum_{i}^{N} a_i \Psi_i(\xi). \tag{1}$$

The orthogonal polynomials can be the Hermite, Legendre, Laguerre, or any other set of orthogonal polynomials, depending on the probabilistic distribution of the random input variables ξ. The physical entities $\mathcal{Y}$ include electromagnetic fields (with uncertainties), particle positions, velocities, and spin vectors.

PCE: Expansion Coefficients

The expansion coefficients can be calculated using intrusive and non-intrusive methods. Non-intrusive methods consider the deterministic code as a black box, *i.e.*, they do not alter the code nor the equations. The expansion coefficients are calculated using multiple calls to the deterministic code either via *projection* or *regression*. Both require a number of N realization pairs $(\xi, \mathcal{Y})$ (see Eq. (1)).

PCE: Projection

Projection requires the evaluation of expectation values and relies on the orthogonality of the polynomials to compute the coefficients in the form of

$$a = \frac{\mathbb{E}\left\{\mathcal{Y}\Psi\right\}}{\mathbb{E}\left\{\Psi^2\right\}} \,. \tag{2}$$

The computation of the expectation values ($\mathbb{E}\{\cdot\}$) necessitates the evaluation of integrals. Quadrature methods are one way to do so, and are commonly used in PCE analyses. Depending on the type of input distribution, the corresponding quadrature rule can be used. The Gauss-Laguerre quadrature for instance, is used in the case of uniformly distributed random variables. It is widely known as non-intrusive spectral projection (NISP).

PCE: Regression

Regression, estimates the coefficients that minimize the functional difference between the estimated response $\hat{\mathcal{Y}}$ and the actual response $\mathcal{Y}$, given by

$$a = \arg\min \left(\mathbb{E} \left\{ \hat{\mathcal{Y}} - \mathcal{Y} \right\}^2 \right) . \tag{3}$$

The solution of Eq. (3), obtained by linear regression, yields

$$a = \left(\Psi^T \cdot \Psi \right) \cdot \Psi \cdot \mathcal{Y}. \tag{4}$$

Beam Tracking Simulations: Equation of Motion

The variational form of the beam and spin dynamic equations is derived using the stochastic Galerkin projection. Neglecting forces other than the electromagnetic ones acting on the charged particles, the beam equations read

$$\begin{aligned} \frac{d}{dt}\vec{v} &= \frac{q}{m\gamma}\left[\vec{E} + \vec{v}\times\vec{B} - \frac{1}{c^2}\vec{v}\left(\vec{v}\cdot\vec{E}\right)\right], \text{ and} \\ \frac{d}{dt}\vec{r} &= \vec{v}\,. \end{aligned} \tag{5}$$

Here, $\vec{E}$ and $\vec{B}$ represent the electric and magnetic fields, and $\vec{v}$ denotes the velocity vector of the particles.

Beam Tracking Simulations: Equation of Motion

The expansion of Eq. (5) in Cartesian coordinates yields a linear system of six coupled ordinary differential equations,

$$\frac{d}{dt}v_x = \frac{q}{m}\left[\frac{1}{\gamma}E_x + \frac{1}{\gamma}v_y B_z - \frac{1}{\gamma}v_z B_y - \frac{1}{c^2\gamma}v_x(\vec{v}\cdot\vec{E})\right]\,, \tag{6a}$$

$$\frac{d}{dt}v_y = \frac{q}{m}\left[\frac{1}{\gamma}E_y + \frac{1}{\gamma}v_z B_x - \frac{1}{\gamma}v_x B_z - \frac{1}{c^2\gamma}v_y(\vec{v}\cdot\vec{E})\right]\,, \tag{6b}$$

$$\frac{d}{dt}v_z = \frac{q}{m}\left[\frac{1}{\gamma}E_z + \frac{1}{\gamma}v_x B_y - \frac{1}{\gamma}v_y B_x - \frac{1}{c^2\gamma}v_z(\vec{v}\cdot\vec{E})\right]\,, \text{ and} \tag{6c}$$

$$\frac{d}{dt}x = v_x\,, \tag{6d}$$

$$\frac{d}{dt}y = v_y\,, \tag{6e}$$

$$\frac{d}{dt}z = v_z\,. \tag{6f}$$

Here, $\vec{v}$ denotes the velocity vector of the particles, q the particle charge, m the mass, γ the Lorentz factor, and $\vec{r}$ the position vector.

Equation of Motion: Variational Form

v_x is expanded as

$$v_x = \sum_i^N {v_x}_i^{(k)} \Psi_i \, , \tag{7}$$

where the ${v_x}_i^{(k)}$ are the chaos expansion coefficients. The superscript (k) is used to identify the expansion coefficients, and also to emphasize that the variables are discretized. The coefficients are calculated according to

$$ {v_x}_i^{(k)} = \left(\Psi^T \cdot \Psi \right) \cdot \Psi \cdot v_{x_0} \, , \tag{8}$$

where v_{x_0} are the initial x-components of the particle velocities. Inserting Eq. (7) into the left-hand side of Eq. (6a), we find

$$\frac{d}{dt} v_x = \frac{d}{dt} \sum_i^N {v_x}_i^{(k)} \Psi_i = \sum_i^N \frac{d}{dt} {v_x}_i^{(k)} \Psi_i \, . \tag{9}$$

Equation of Motion: Variational Form

The **stochastic Galerkin projection** is applied by multiplying Eq. (9) with Ψ_l and taking the expectation value $\mathbb{E}\{\cdot\}$, which gives

$$\begin{aligned} \mathbb{E}\left\{\sum_{i}^{N}\frac{d}{dt}{v_x}_i^{(k)}\Psi_i\Psi_l\right\} &= \sum_{i}^{N}\frac{d}{dt}{v_x}_i^{(k)}\mathbb{E}\left\{\Psi_i\Psi_l\right\} \\ &= \sum_{i}^{N}\frac{d}{dt}{v_x}_i^{(k)}\langle\Psi_i\Psi_l\rangle \\ &= \sum_{i}^{N}\frac{d}{dt}{v_x}_i^{(k)}\langle\Psi_i^2\rangle\delta_{il}\,. \end{aligned} \tag{10}$$

Here δ_{il} is the Kronecker delta which results from the orthogonality of the polynomials.

Equation of Motion: Variational Form

The electric field is also represented stochastically as by the finite series

$$E_x = \sum_{i}^{N} {e_x}_i^{(k)} \Psi_i \,. \tag{11}$$

The Cartesian components of the electric and magnetic fields ($\vec{E}$ and $\vec{B}$) are functions of the position vector $\vec{r}$, *e.g.*, $\vec{E}_x(\vec{r})$, $\vec{B}_x(\vec{r})$, etc. The dependence of the field components on position, *e.g.*, $\vec{E}_x(\vec{r}) = \vec{E}_x(x, y, z)$, does not pose a problem for the PCE method as long as the input variables (*e.g.*, $\vec{r}$ and $\vec{v}$) are *independent*

Equation of Motion: Variational Form

The Lorentz factor γ constitutes also a stochastic variable. Unfortunately, it appears in the denominator of all terms in Eq. (5). To solve this problem, $1/\gamma$ is expanded instead of γ. Let α be defined as

$$\alpha = \frac{1}{\gamma}\,, \tag{12}$$

then α is expanded as

$$\alpha = \sum_{i}^{N} \alpha_i^{(k)} \Psi_i\,. \tag{13}$$

Equation of Motion: Variational Form

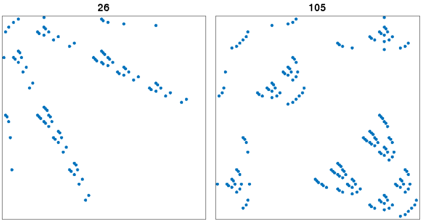
The stochastic Galerkin projection is applied by multiplying the product of Eqs. (11) and (13) by Ψ_k, and subsequently calculating the expectation value $\mathbb{E}\{\cdot\}$. It thus follows that

$$\begin{aligned}\mathbb{E}\left\{\sum_i^N {e_x}_i^{(k)}\Psi_i \sum_j^N \alpha_j^{(k)}\Psi_j\Psi_l\right\} &= \sum_i^N\sum_j^N {e_x}_i^{(k)}\alpha_j^{(k)}\langle\Psi_i\Psi_j\Psi_l\rangle \\ &= \sum_i^N\sum_j^N \alpha_i^{(k)}{e_x}_j^{(k)} C_{ijl}.\end{aligned} \tag{14}$$

The $C_{ijl} = \langle\Psi_i\Psi_j\Psi_l\rangle$ tensor constitutes a sparse rank-3 tensor.

C_{ijl} Tensor

C_{ijl} is a computationally CPU-extensive operation, but fortunately, it needs to be computed only once. It can be stored and re-used when required. Although the multiplications of the PCE coefficients involve the C_{ijl} term, this arithmetic operation does not introduce any computational overhead as C_{ijl} is sparse.



With the $m = 5$ dimensional problem and an expansion order of $p = 4$, the number of basis functions is $P = 126$, which results in a $(126 \times 126 \times 126)$ C_{ijl} tensor.

Equation of Motion: Variational Form

The next term of Eq. (6a), the product of α, velocity v_y, and magnetic field B_z presents a more complicated situation, because it involves multiple polynomials

$$
\begin{aligned}
v_y &= \sum_i^N {v_y}_i^{(k)} \Psi_i \,, \\
B_z &= \sum_i^N {b_z}_i^{(k)} \Psi_i \,,
\end{aligned} \tag{15}
$$

where ${v_y}_i^{(k)}$ and ${b_z}_i^{(k)}$ are the expansion coefficients of v_y and B_z, respectively. The multiplication of the three sums yields

$$
\alpha v_y B_z = \sum_i^N \sum_j^N \sum_k^N \alpha_i^{(k)} {v_y}_j^{(k)} {b_z}_k^{(k)} \Psi_i \Psi_j \Psi_k \,. \tag{16}
$$

Equation of Motion: Variational Form

By applying the stochastic Galerkin projection to Eq. (16), it follows that

$$
\begin{aligned}
\mathbb{E}\left\{\alpha v_y B_z \Psi_l\right\} &= \sum_i^N \sum_j^N \sum_k^N \alpha_i^{(k)} {v_y}_j^{(k)} {b_z}_k^{(k)} \langle \Psi_i \Psi_j \Psi_k \Psi_l \rangle \\
&= \sum_i^N \sum_j^N \sum_k^N \alpha_i^{(k)} {v_y}_i^{(k)} {b_z}_j^{(k)} D_{ijkl} \,.
\end{aligned}
\tag{17}
$$

D_{ijkl} is similar to C_{ijl}, but it constitutes a rank-4 tensor. The case for the third term of Eq. (6a) yields

$$
\begin{aligned}
\mathbb{E}\left\{\alpha v_z B_y \Psi_k\right\} &= \sum_i^N \sum_j^N \sum_k^N \alpha_i^{(k)} {v_z}_j^{(k)} {b_y}_k^{(k)} \langle \Psi_i \Psi_j \Psi_k \Psi_l \rangle \\
&= \sum_i^N \sum_j^N \sum_k^N \alpha_i^{(k)} {v_z}_j^{(k)} {b_y}_k^{(k)} D_{ijkl} \,.
\end{aligned}
\tag{18}
$$

Equation of Motion: Variational Form

The last term of the right hand side of Eq. (6a), *i.e.*,

$$\frac{1}{c^2}\alpha v_x \left(\vec{v} \cdot \vec{E}\right) \tag{19}$$

is yet more complicated, because it involves a scalar product. The scalar product operator multiplies the operands component-wise before summing them up. These operands, however, are PC coefficients. The corresponding multiplication is in fact a Galerkin one, which involves a series of double products given by

$$\vec{v} \cdot \vec{E} = \sum_{i}^{3} \sum_{j}^{N} \sum_{k}^{N} v_{i_j}^{(k)} e_{i_k}^{(k)} \Psi_j \Psi_k \,. \tag{20}$$

Equation of Motion: Variational Form

This means that Eq. (20) requires the stochastic Galerkin projection to compute a rank-5 tensor, which makes the method highly inefficient. In order to solve this problem, a **pseudo-spectral method** is used. The Galerkin projection is applied first to the auxiliary variable g_l (the one representing the scalar product), and then secondly to the full product in Eq. (19). This way, the rank-4 tensor product, introduced above in Eq. (17), can be used. In particular, g_l reads

$$g_l = \mathbb{E}\left\{\left(\vec{v}\cdot\vec{E}\right)\Psi_l\right\} = \sum_i^3 \sum_j^N \sum_k^N v_{i_j}^{(k)} e_{i_k}^{(k)} C_{ijl}\,, \qquad (21)$$

where the subscript l here constitutes a free variable. And then, by applying the stochastic Galerkin projection, it follows that

$$\mathbb{E}\left\{\alpha v_x\left(\vec{v}\cdot\vec{E}\right)\Psi_l\right\} = \sum_i^N \sum_j^N \sum_k^N \alpha_i^{(k)} v_{x_j}^{(k)} g_k^{(k)} D_{ijkl}\,. \qquad (22)$$

T-BMT equation

The spin dynamics in an electromagnetic storage ring with non-vanishing EDM is described by the generalized T-BMT equation which reads

$$\frac{d}{dt}\vec{S} = \left(\vec{\Omega}^{\mathrm{MDM}} + \vec{\Omega}^{\mathrm{EDM}}\right) \times \vec{S}\,. \tag{23}$$

Here, $\vec{S}$ denotes the particle spin, and $\vec{\Omega}^{\mathrm{EDM}}$ and $\vec{\Omega}^{\mathrm{MDM}}$ are the angular velocities associated with the magnetic (MDM) and electric dipole moments (EDM). $\vec{\Omega}^{\mathrm{MDM}}$ and $\vec{\Omega}^{\mathrm{EDM}}$ are defined as

$$\begin{aligned}
\vec{\Omega}^{\mathrm{MDM}} &= -\frac{q}{m\gamma}\Bigg[(1+G\gamma)\,\vec{B} + \left(G\gamma + \frac{\gamma}{1+\gamma}\right)\frac{\vec{E}\times\vec{\beta}}{c} \\
&\quad - \frac{G\gamma^2}{\gamma+1}\vec{\beta}\left(\vec{\beta}\cdot\vec{B}\right)\Bigg]\,, \qquad (24) \\
\vec{\Omega}^{\mathrm{EDM}} &= -\frac{q}{m}\frac{\eta}{2}\left[\frac{\vec{E}}{c} + \vec{\beta}\times\vec{B} - \frac{\gamma}{\gamma+1}\vec{\beta}\left(\vec{\beta}\cdot\frac{\vec{E}}{c}\right)\right].
\end{aligned}$$

T-BMT Equation: Variational Form

Rewriting, *e.g.*, ${\Omega_y^{\mathrm{MDM}}}_i^{(k)}$ in terms of the individual components, is equivalent to the following expression

$$
\begin{aligned}
&\sum_i^N {\Omega_y^{\mathrm{MDM}}}_i^{(k)} \\
&= -\frac{q}{m}\Bigg[\sum_i^N\sum_j {f_1}_i^{(k)} {b_y}_j^{(k)} C_{ijl} \\
&\quad + \sum_i^N\sum_j\sum_k \left({f_2}_i^{(k)} {e_z}_i^{(k)} {\beta_x}_j^{(k)} D_{ijkl} - {f_2}_i^{(k)} {e_x}_i^{(k)} {\beta_z}_j^{(k)} D_{ijkl} \right) \\
&\quad - \sum_i^N\sum_j^N\sum_k^N {f_3}_i^{(k)} {\beta_y}_j^{(k)} h_k^{(k)} D_{ijkl} \Bigg] ,
\end{aligned} \tag{25}
$$

where

$$
h_l = \mathbb{E}\left\{ \left(\vec{\beta} \cdot \vec{B} \right) \Psi_l \right\} = \sum_i^3\sum_j^N\sum_k^N {\beta_i}_j^{(k)} {b_i}_k^{(k)} C_{ijl} \, . \tag{26}
$$

SGM Validation

At the final stage, the performance of the SGM must be evaluated quantitatively, with the help of an adequate error analysis. Due to time and position dependencies, the error calculation involves either the mean value (μ) or the standard deviation (σ) of the quantity under investigation, denoted in the following by ζ. The corresponding errors are called ϵ_μ and ϵ_σ, respectively, and are defined as

$$\epsilon_\mu(t) = \left| \frac{\bar{\zeta}(t) - \bar{\hat{\zeta}}(t)}{\bar{\zeta}(t)} \right|, \text{ and} \tag{27a}$$

$$\epsilon_\sigma(t) = \left| \frac{\sigma[\zeta(t)] - \sigma[\hat{\zeta}(t)]}{\sigma[\zeta(t)]} \right|. \tag{27b}$$

Here, ζ may refer to either the position, velocity or spin vector, while $\hat{\zeta}$ denotes the value estimated using the SGM. The exact initial conditions are inserted into both the MC and the SGM solver, so that the solutions can be directly compared on a particle-by-particle basis.

SGM Validation

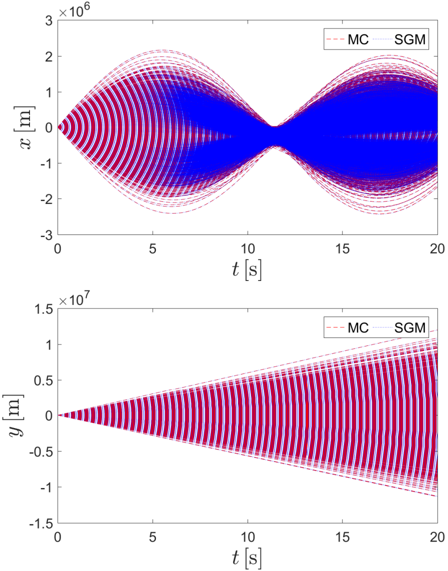
When the dynamics includes electromagnetic fields that are functions of position, time, or frequency, the stochastic expansion coefficients may evolve as a function of time, position, etc. This adds another level of complexity that the SGM must be able to cope with. As a consequence, the performance criterion in Eq. (27) must be modified to account for position (or other) dependencies as well,

$$\epsilon_\mu(z) = \left| \frac{\bar{\zeta}(z) - \bar{\hat{\zeta}}(z)}{\bar{\zeta}(z)} \right|, \text{ and} \tag{28a}$$

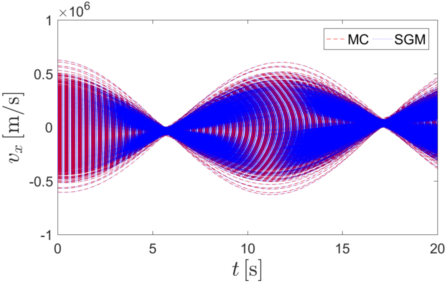
$$\epsilon_\sigma(z) = \left| \frac{\sigma[\zeta(z)] - \sigma[\hat{\zeta}(z)]}{\sigma[\zeta(z)]} \right|. \tag{28b}$$

Here, ζ may refer either to the position, velocity or spin dependence, and $\hat{\zeta}$ constitutes the corresponding estimated value using the SGM, similar to Eq. (27).

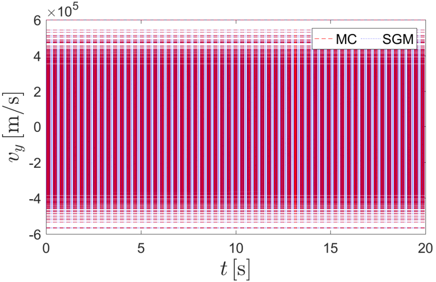
SGM Results



SGM Results

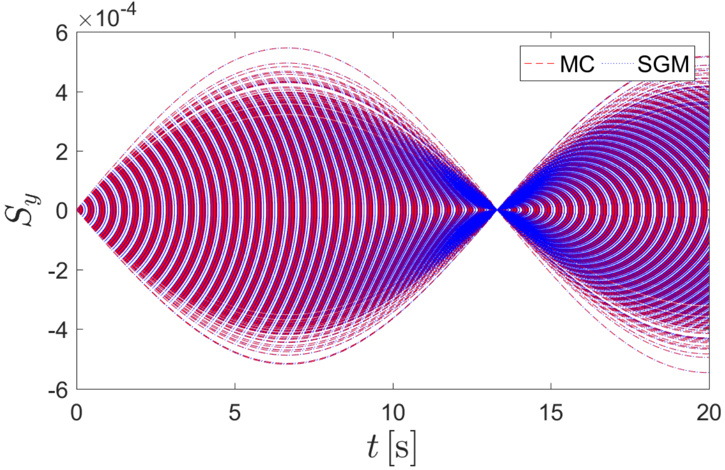


$\times 10^6$
1
0.5
0
-0.5
-1
v_x [m/s]
0
5
10
15
20
t [s]
MC
SGM

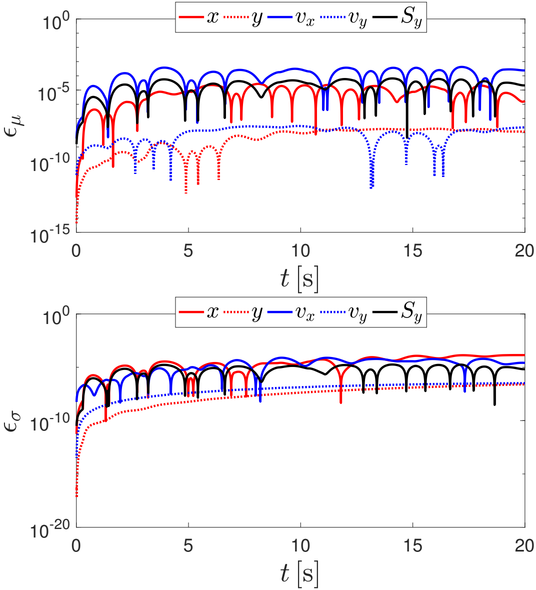


$\times 10^5$
6
4
2
0
-2
-4
-6
v_y [m/s]
0
5
10
15
20
t [s]
MC
SGM

SGM Results

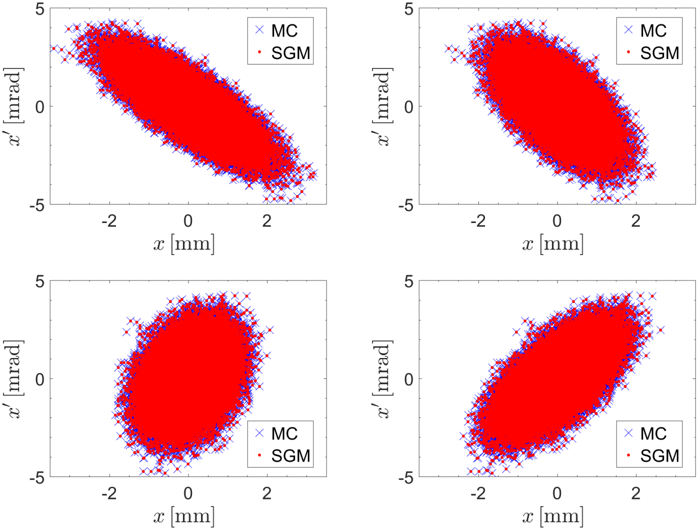


SGM Results

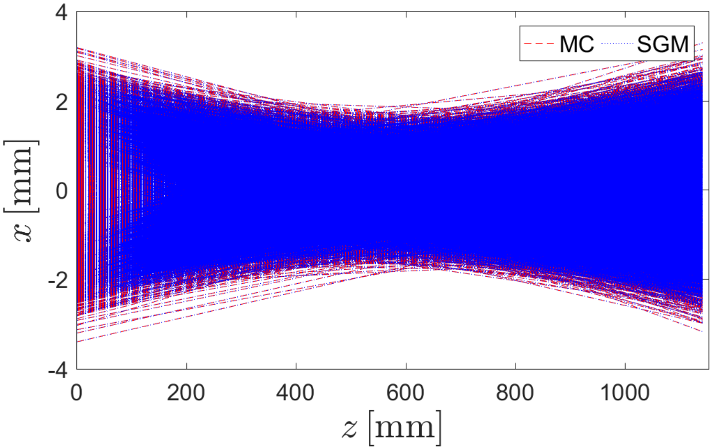


x y v_x v_y S_y
10^{0}
10^{-5}
10^{-10}
10^{-15}
ϵ_μ
0 5 10 15 20
t [s]
x y v_x v_y S_y
10^{0}
10^{-10}
10^{-20}
ϵ_σ
0 5 10 15 20
t [s]

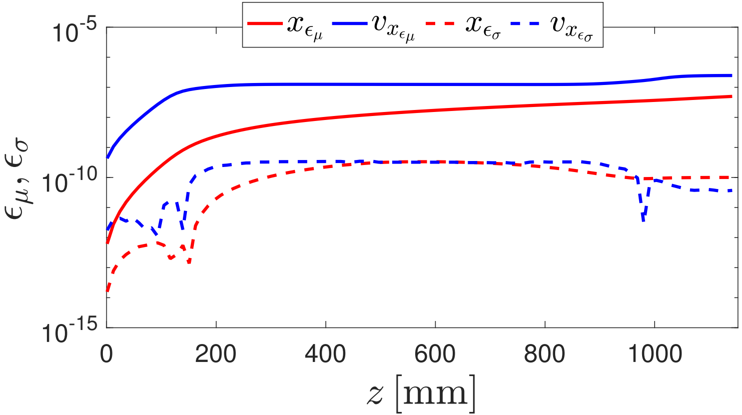
SGM Results



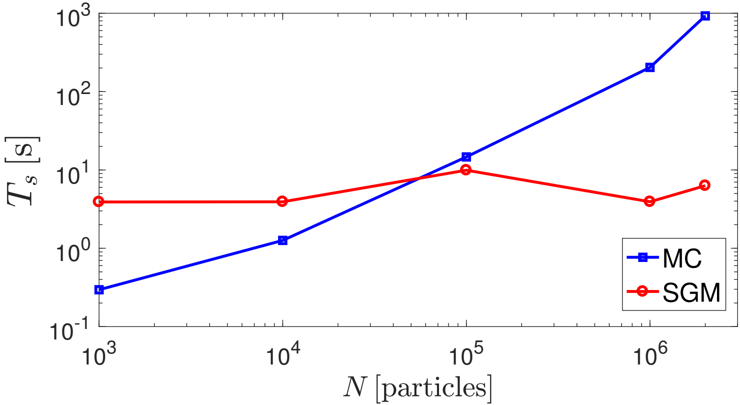
SGM Results: Real Fields



SGM Results: Real Fields



SGM vs MC: Simulation Time



Comparison of the simulation time required for the parallelized MC and the stochastic Galerkin method (SGM). For particle numbers below about 10^5, the methods are comparable. For larger particle numbers with a constant expansion order of $p = 4$, the time required for the SGM stays constant, while the demand for the MC increases exponentially.