Spin dynamics in modern electron storage rings: Computational aspects

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Outline

1. The Reduced Bloch equation in 1,2 and 3 Degrees of Freedom
2. Numerical approach
3. Numerical results

The Reduced Bloch Equation in 3 Degrees of Freedom

The Reduced Bloch Equation in 3 Degrees of Freedom (DOF) for polarization density $\vec{\eta}$ is

$$\partial_\theta \vec{\eta} = \left(-\sum_{j=1}^{6} \partial_{y_j} \Big(\mathcal{A}(\theta) y \Big)_j + \frac{1}{2} \omega_Y(\theta) \partial_{y_6}^2 d + \Omega_Y(\theta, y) \right) \vec{\eta}.$$

We want to compute polarization: $\vec{P}(t) = \int \vec{\eta} dy$.
A cost of a numerical simulation will scale no better then $\mathcal{O}(N^6)$ per time step when each y_i is discretized on a grid with N grid points.

The Averaged Reduced Bloch equations in 2 DOF Flat Ring

$$\partial_\theta \vec{\eta} = \overbrace{-\sum_{i=1}^{4} \partial_{w_i} \left[(\overline{\mathcal{D}} w)_i \vec{\eta} \right]}^{\text{Drift}} + \overbrace{\frac{\varepsilon}{2} \left(\overline{\mathcal{E}}_{11} \Delta_{1,2} + \overline{\mathcal{E}}_{33} \Delta_{3,4} \right) \vec{\eta}}^{\text{Diffusion}}$$

$$\underbrace{-\varepsilon \sum_{i=1}^{4} \left(\overline{\mathcal{D}}_{5i} w_i \right) \mathcal{J}_2 \vec{\eta} - \frac{\varepsilon}{2} \overline{\mathcal{E}}_{55} \vec{\eta} + \varepsilon \sum_{i=1}^{4} \overline{\mathcal{E}}_{i5} \partial_{w_i} \mathcal{J}_2 \vec{\eta},}_{\text{Spin}} \qquad \mathcal{J}_2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

The exact solution can be found to compare with the numerical solution.

The Flat Ring model reduces to the 1 DOF model

- Heavily studied since 90s.
- Exact solution found.

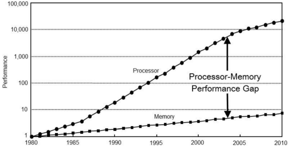
2 DOF reduces to

$$\partial_t \vec{\eta} = \overbrace{\varepsilon\left(\partial_{w_1}(w_1\vec{\eta}) + \partial_{w_2}(w_2\vec{\eta})\right)}^{\text{Drift}} + \overbrace{\frac{\varepsilon}{4}\Delta\vec{\eta}}^{\text{Diffusion}}$$
$$\underbrace{-\varepsilon g w_1 \mathcal{J}_2 \vec{\eta} - \frac{\varepsilon}{2} g \mathcal{J}_2 \partial_{w_1}\vec{\eta} - \frac{\varepsilon}{4} g^2 \vec{\eta}}_{\text{Spin}}.$$

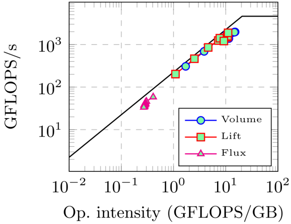
with $\varepsilon \approx 0.08$ and $g \approx 2.07$ (Parameters from HERA, DESY).

Why we use the high order methods?

High arithmetic intensity



Computer Architecture: A Quantitative Approach by John L. Hennessy, David A. Patterson, Andrea C. Arpaci-Dusseau.



Chan & Warburton, SISC, 2017.

- Points per wavelength don't give us any other choice.
- If error tolerance is set to 1%.

$$
\begin{aligned}
PPW_2(j) &= 64j^{1/2}, \\
PPW_4(j) &= 13j^{1/4}, \\
PPW_6(j) &= 8j^{1/6}.
\end{aligned}
$$

Kreiss & Oliger, Tellus 1972

Second order vs sixth order method.
Grid points in 1D, 640 vs 16.
Grid points in 3D, 262,144,000 vs 4,096.

Reduced Bloch equation in polar coordinates

$$\partial_t \vec{\eta} = \varepsilon \Big(\partial_{w_1}(w_1 \vec{\eta}) + \partial_{w_2}(w_2 \vec{\eta}) \Big) + \frac{\varepsilon}{4} \Delta \vec{\eta} - \varepsilon g w_1 \mathcal{J} \vec{\eta} - \frac{\varepsilon}{2} g \mathcal{J} \partial_{w_1} \vec{\eta} - \frac{\varepsilon}{4} g^2 \vec{\eta}.$$

$$w_1 = r\cos\varphi, \quad w_2 = r\sin\varphi$$

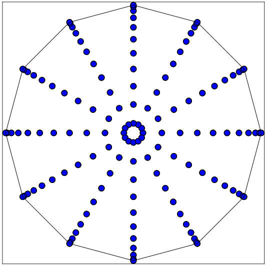
$$\partial_t \vec{\eta} = \frac{\varepsilon}{4} \Big[\Big((8 - g^2) + (4r + r^{-1})\partial_r + \partial_r^2 + r^{-2}\partial_\varphi^2 \Big) \vec{\eta} - 2g\mathcal{J} \Big(2r\cos\varphi + \cos\varphi \partial_r - r^{-1}\sin\varphi \partial_\varphi \Big) \vec{\eta} \Big].$$

Discretization

We seek approximations to η on a Chebyshev grid in r and a uniform grid in φ,

$$r_i = -\cos\left(\frac{\pi i}{n_r}\right), \qquad i = 0, \ldots, n_r,$$

$$\varphi_j = j\frac{2\pi}{n_\varphi}, \qquad j = 1, \ldots, n_\varphi.$$

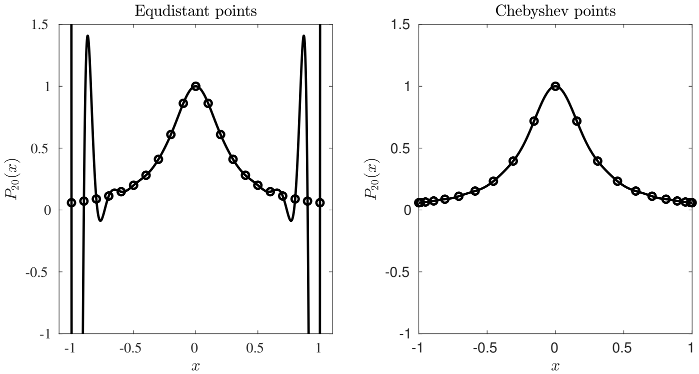


Why we use a Chebyshev discretization?

- Chebyshev points are

$$x_i = \cos(i\pi/N), \quad i = 0, \dots, N.$$

- Minimize the ∞-norm of the interpolation error.



Discrete Fourier transform in φ

$$\partial_t \vec{\eta} = \frac{\varepsilon}{4}\Bigg[\Bigg((8-g^2)+(4r+r^{-1})\partial_r+\partial_r^2+r^{-2}\partial_\varphi^2\Bigg)\vec{\eta} \\ -2g\mathcal{J}\Bigg(2r\cos\varphi+\cos\varphi\partial_r-r^{-1}\sin\varphi\partial_\varphi\Bigg)\vec{\eta}\Bigg].$$

Truncated Fourier series in the φ direction:

$$\eta(r_i,\varphi_j,t) \approx \sum_{k=-n_{\varphi/2}+1}^{n_\varphi/2} \hat{\eta}(r_i,k,t)e^{-\imath k\varphi_j}.$$

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$$-2g\mathcal{J}\bigg(2r\cos\varphi+\cos\varphi\partial_r-r^{-1}\sin\varphi\partial_\varphi\bigg)\vec{\eta}\Bigg].$$

Truncated Fourier series in the φ direction:

$$\eta(r_i,\varphi_j,t)\approx\sum_{k=-n_{\varphi/2}+1}^{n_\varphi/2}\hat{\eta}(r_i,k,t)e^{-\imath k\varphi_j}.$$

For the kth Fourier mode we determine $\hat{\eta}(r,k,t)$ from

$$\partial_t\hat{\eta}_l=\frac{\varepsilon}{4}\Bigg[\bigg((8-g^2)+(4r+r^{-1})\partial_r+\partial_r^2-r^{-2}k^2\bigg)\hat{\eta}_l$$
$$+gJ_{lm}\bigg((2r+\partial_r)(\hat{\eta}_m^-+\hat{\eta}_m^+)-r^{-1}\left((k\hat{\eta}_m)^--(k\hat{\eta}_m)^+\right)\bigg)\Bigg],$$
$$\hat{\eta}_l^{\,-}=\hat{\eta}_l(r,k-1,t),\quad \hat{\eta}_l^{\,+}=\hat{\eta}_l(r,k+1,t).$$

Numerical differentiation of function $f(x)$

1. Let p be the unique interpolant of order N with

$$p(x_i) = v_i = f(x_i), \quad 0 \leq i \leq N.$$

2. Set $w_i = p'(x_i)$.

This operation can be expressed as matrix-vector product [2]

$$w = Dv.$$

[2] B. Fornberg, "Classroom Note: Calculation of Weights in Finite Difference Formulas", *SIAM Review*, vol. 40(3), pp. 685–691, 1998.

Numerical scheme

- *Grid function* $\hat{u}_1(k,t)$:

$$\hat{u}_1(k,t) = [\hat{u}_1(r_0,k,t), \ldots, \hat{u}_1(r_{n_r},k,t)]^T$$

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- Describes the first component of $\hat{\eta}$.

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- Describes the first component of $\hat{\eta}$.
- Evolved by a system of ODE

$$\frac{d\,\hat{u}_1(k,t)}{dt} = \frac{\varepsilon}{4}\left[F_I^k(\hat{u}_1) + F_E^k(\hat{u}_2)\right].$$

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$$\frac{d\,\hat{u}_1(k,t)}{dt} = \frac{\varepsilon}{4}\left[F_I^k(\hat{u}_1) + F_E^k(\hat{u}_2)\right].$$

- F_I and F_E are linear operators - discretized Fokker-Planck operator and spin terms

$$F_I(\hat{u}_1) = \left((8-g^2)I + (4R+R^{-1})D_1 + D_2 - R^{-2}k^2\right)\hat{u}_1,$$
$$F_E(\hat{u}_2) = \left((2R+D_1)(\hat{u}_2^+ + \hat{u}_2^-) - R^{-1}((k\hat{u}_2)^- - (k\hat{u}_2)^+\right).$$

March in time via implicit-explicit method

Let $\hat{u}^{\nu}(k) = \hat{u}(k, \nu\Delta t)$ then, for each mode, we compute

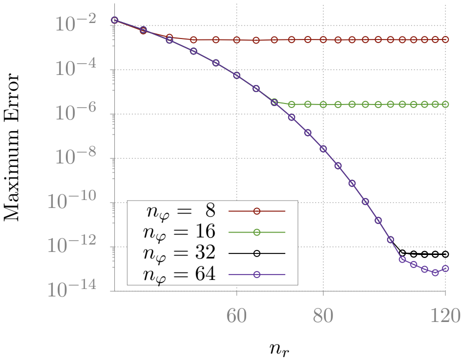
$$\hat{u}^{\nu+1} = \hat{u}^{\nu} + \sum_{s=1}^{N} \gamma_s \mathbf{k}_s,$$

$$\mathbf{k}_s = \frac{\varepsilon \Delta t}{4} \left[F_I \left(\hat{u}^{\nu} + \sum_{l=1}^{s} \alpha_{sl} \mathbf{k}_l \right) + F_E \left(\hat{u}^{\nu} + \sum_{l=1}^{s-1} \beta_{sl} \mathbf{k}_l \right) \right].$$

Spectral convergence

$$\eta(t,w) = \frac{2}{\pi} e^{\Sigma_2} \begin{pmatrix} \cos(\psi_0 + \Sigma_1 w_1) \\ \sin(\psi_0 + \Sigma_1 w_1) \end{pmatrix} e^{-2(w_1^2+w_2^2)},$$

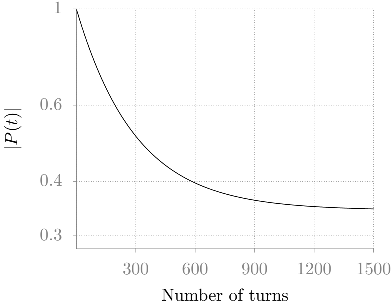
$$\Sigma_1(t) = -g(1-e^{-\varepsilon t}), \quad \Sigma_2(t) = \frac{g^2}{8}(e^{-2\varepsilon t} - 1).$$



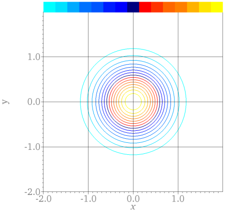
Polarization comes for free

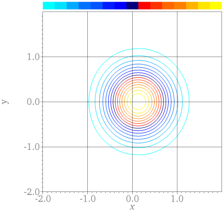
- $\vec{P}(t) = \int \vec{\eta}(t, w) dw$
- Chebyshev points are quadrature points - just sum up the weighted grid function values.
- For initial condition

$$\vec{\eta}_0(w) = \frac{2}{\pi} \begin{pmatrix} \cos \psi_0 \\ \sin \psi_0 \end{pmatrix} e^{-2(w_1^2 + w_2^2)},$$



Numerical results





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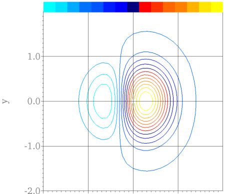

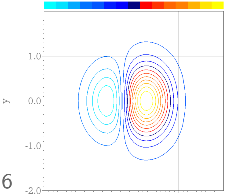

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