Rapid Integration Over History in Self-consistent 2D CSR Modeling

Klaus Heinemann, David Bizzozero, James A. Ellison, Stephen Lau

Dept. Mathematics & Statistics, University of New Mexico

Gabriele Bassi

Brookhaven National Laboratory, Upton, Long Island, New York

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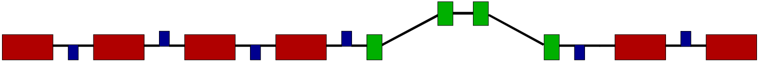
(1) Vlasov-Maxwell approach to bunch compressor

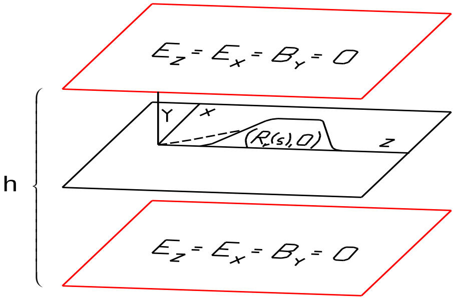
(2) Current paradigm:
- Sheet bunch moving in the midplane between the two shielding plates
- Monte Carlo Particle (MCP) algorithm with MPI-FORTRAN code VM3@A (**V**lasov-**M**axwell **M**onte-Carlo **M**ethod at **A**lbuquerque)

(3) Modification of current paradigm: Get rid of integration over history by doing Fourier transform of field + approximation of Bessel function J_0

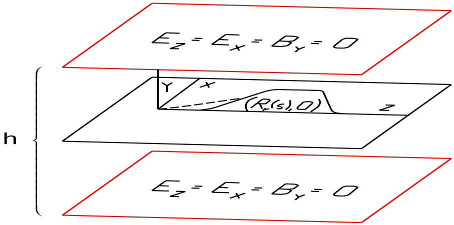
(4) Future paradigm: Direct time integration of the VM system of PDEs, e.g., Discontinuous Galerkin method



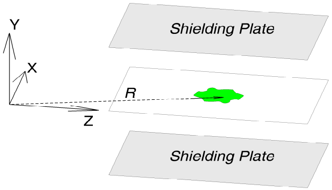
Proposed layout of FERMI@Elettra first bunch compressor system. The four dipoles are in green.



- Setup: 4-dipole bunch compressor with two perfectly conducting shielding plates parallel to $Y = 0$ plane
- Vlasov-Maxwell approach: 6D phase space density $f(\mathbf{R}, Y, \mathbf{P}, P_Y, u)$ satisfying Vlasov equation for self field $\mathbf{E}(\mathbf{R}, Y, u), \mathbf{B}(\mathbf{R}, Y, u)$ with $\mathbf{R} = (Z, X), \mathbf{P} = (P_Z, P_X), u = ct$
- Self field $\mathbf{E}, \mathbf{B}$ satisfies Maxwell's equations for charge/current densities $\rho_f, \mathbf{j}_f$ of f ("mean field" approach to $\mathbf{E}, \mathbf{B}$)



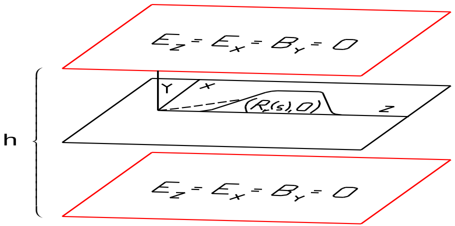
- Self field solves initial-boundary problem for wave equation:
  - Wave Equation: $\Box \mathbf{E} = \mathbf{S}_E(\mathbf{R}, Y, u)$, $\Box \mathbf{B} = \mathbf{S}_B(\mathbf{R}, Y, u)$ where $\Box = \frac{\partial^2}{\partial X^2} + \frac{\partial^2}{\partial Y^2} + \frac{\partial^2}{\partial Z^2} - \frac{\partial^2}{\partial u^2}$ and $\mathbf{S}_E, \mathbf{S}_B$ determined by $\rho_f, \mathbf{j}_f$
  - Dirichlet condition on shielding plates for E_Z, E_X, B_Y
  - Neumann condition on shielding plates for E_Y, B_X, B_Z
  - Neglect initial self field $\Longrightarrow$ $\mathbf{E}, \mathbf{B}, \frac{\partial \mathbf{E}}{\partial u}, \frac{\partial \mathbf{B}}{\partial u}$ vanish at $u = 0$
- Brute force method: Compute f in whole phase space and compute $\mathbf{E}, \mathbf{B}$ in whole configuration space
- More efficient method than brute force method needed: See below!



- Sheet bunch inside midplane between two shielding plates

$$f(\mathbf{R}, Y, \mathbf{P}, P_Y, u) = \delta(Y)\delta(P_Y)f_{sheet}(\mathbf{R}, \mathbf{P}, u)$$
$$\rho(\mathbf{R}, Y, u) = \delta(Y)\rho_{sheet}(\mathbf{R}, u)$$
$$\mathbf{j}(\mathbf{R}, Y, u) = \delta(Y)\mathbf{j}_{sheet}(\mathbf{R}, u)$$

- f_{sheet} simulated by particles (not computed!) $\longrightarrow$ Monte Carlo Particle (MCP) algorithm with MPI-FORTRAN code VM3@A
- $\rho_{sheet}, \mathbf{j}_{sheet}$ computed by density estimation



Sheet bunch $\Longrightarrow$

- $\mathbf{E}, \mathbf{B}$ only needed in $Y = 0$ plane
- E_Y, B_X, B_Z vanish in $Y = 0$ plane
- E_Z, E_X, B_Y vanish on shielding plates (Dirichlet condition)
- Abbreviate $\mathbf{F}(\mathbf{R}, u) := (E_Z(\mathbf{R}, 0, u), E_X(\mathbf{R}, 0, u), B_Y(\mathbf{R}, 0, u))$

- Initial boundary problem of wave equation gives

$$\mathbf{F} = \mathbf{F}_0 + \mathbf{F}_1 \ ,$$

where $\mathbf{F}_0$ is the nonshielding contribution:

$$\mathbf{F}_0(\mathbf{R}, u) = \frac{-1}{4\pi} \int_0^u \int_{-\pi}^{\pi} dv d\theta \mathbf{S}(\mathbf{R} + \mathbf{e}(\theta)(u - v), v)$$

with $\mathbf{e}(\theta) = (\cos\theta, \sin\theta)$ and source $\mathbf{S}$ is determined by $\rho_{sheet}, \mathbf{j}_{sheet}$ and $\mathbf{F}_1$ is the nonshielding term

- Remarks:
  - v-integral in self field involves history of $\mathbf{S}$

- Remarks (continued):
  - Nonshielding term $\mathbf{F}_0$ often sufficient for applications
  - For v-integration we use adaptive integrator (Gauss-Kronrod)
  - θ integration is done with trapezoidal rule
  - Evolution of source governed by Vlasov equation $\Longrightarrow$ use Monte Carlo particle method in accelerator coordinates using a density estimation procedure (e.g. kernel density estimation with a product of Epanechnikov kernels)
  - Self field computation is most time consuming part because of v-integral over bunch history - flop count per time step is $O(N_X N_Z N_v N_\theta)$ where $N_X N_Z$ is number of field grid points, $N_v N_\theta$ is number of integration grid points
  - To improve efficiency, see below

Modification of current paradigm - Part I

- In the absence of shielding

$$\mathbf{F}_0(\mathbf{R},u)=\frac{-1}{4\pi}\int_0^u\int_{-\pi}^{\pi}dvd\theta\mathbf{S}(\mathbf{R}+\mathbf{e}(\theta)(u-v),v)$$

- Fourier transform in $\mathbf{R}$ of $\mathbf{S}(\mathbf{R},u)$ and $\mathbf{F}(\mathbf{R},u)$:

$$\tilde{\mathbf{S}}(\mathbf{k},u)=\frac{1}{2\pi}\int_{\mathbb{R}^2}d\mathbf{R}\exp(-i\mathbf{k}\cdot\mathbf{R})\mathbf{S}(\mathbf{R},u)$$

$$\tilde{\mathbf{F}}_0(\mathbf{k},u)=\frac{1}{2\pi}\int_{\mathbb{R}^2}d\mathbf{R}\exp(-i\mathbf{k}\cdot\mathbf{R})\mathbf{F}_0(\mathbf{R},u)$$

- $\Longrightarrow \widetilde{\mathbf{F}}_0(\mathbf{k},u)=-\frac{1}{2}\int_0^u dv\widetilde{\mathbf{S}}(\mathbf{k},v)J_0((u-v)|\mathbf{k}|)$
  where J_0 is zeroth order Bessel function of first kind and $|\mathbf{k}|=\sqrt{k_X^2+k_Z^2}$

Modification of current paradigm - Part II

- Get rid of integral over history of bunch by approximating J_0:

$$J_0(v) \approx \sum_{n=1}^{N_E} \alpha_n \exp(\beta_n v)$$

- $\Longrightarrow$ $\widetilde{\mathbf{F}}_0(\mathbf{k}, u) \approx \sum_{n=1}^{N_E} \alpha_n \widetilde{\mathbf{F}}_n(\mathbf{k}, u)$ where

$$\widetilde{\mathbf{F}}_n(\mathbf{k}, u) = -\frac{1}{2} \int_0^u dv \widetilde{\mathbf{S}}(\mathbf{k}, v) \exp(\beta_n (u - v)|\mathbf{k}|)$$

- $\Longrightarrow$ $\frac{\partial \widetilde{\mathbf{F}}_n}{\partial u} = \beta_n |\mathbf{k}| \widetilde{\mathbf{F}}_n - \frac{1}{2} \widetilde{\mathbf{S}}(\mathbf{k}, u)$

- Thus we get rid of history of bunch ($\Delta > 0$ is time step):

$$\widetilde{\mathbf{F}}_n(\mathbf{k}, u) = \exp(\beta_n \Delta |\mathbf{k}|) \widetilde{\mathbf{F}}_n(\mathbf{k}, u - \Delta) \\ -\frac{1}{2} \int_{u-\Delta}^{u} dv \widetilde{\mathbf{S}}(\mathbf{k}, v) \exp(\beta_n (u - v) |\mathbf{k}|)$$

- Remarks:
  - Above formula is the center piece of modified paradigm - it effectively removes the v-integration over bunch history
  - At a point in code where we compute $\mathbf{F}(\mathbf{R}, u)$, we know the particle phase space positions. In addition in the modified paradigm we will also know the $\widetilde{\mathbf{F}}_n(\mathbf{k}, u - \Delta)$ and $\widetilde{\mathbf{S}}(\mathbf{k}, u - \Delta)$
  - We first compute $\mathbf{S}(\mathbf{R}, u)$ from the particle positions, $\widetilde{\mathbf{S}}(\mathbf{k}, u)$ by FFT and then $\widetilde{\mathbf{F}}_n(\mathbf{k}, u)$ from above formula
  - $\widetilde{\mathbf{S}}(\mathbf{k}, v)$ slowly varying $\Longrightarrow$ above integral can be done after linear interpolation of $\widetilde{\mathbf{S}}(\mathbf{k}, v)$ using $\widetilde{\mathbf{S}}(\mathbf{k}, \cdot)$ at $u - \Delta$ and u
  - From $\widetilde{\mathbf{F}}_n(\mathbf{k}, u)$ we find $\mathbf{F}(\mathbf{R}, u)$ by an inverse FFT and then evolve particles to $u + \Delta$.
  - For nonuniform grid, NFFT will be used instead of FFT

- Remarks (continued):
  - The coefficients α_n and β_n in our approximation:

$$J_0(v) \approx A(v) \equiv \sum_{n=1}^{N_E} \alpha_n \exp(\beta_n v)$$

are obtained from an optimization problem.
  - In fact taking Laplace transform one obtains:

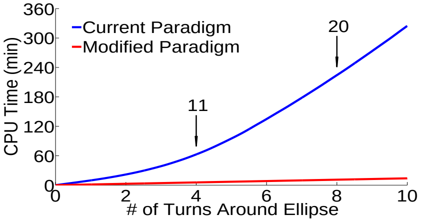
$$\widehat{J}_0(s) = \frac{1}{\sqrt{s^2+1}} \approx \sum_{n=1}^{N_E} \frac{\alpha_n}{s-\beta_n} = \hat{A}(s)$$

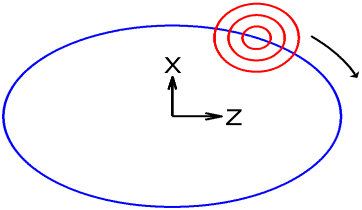
whence, for given N_E one is interested in α_n, β_n which satisfy

$$\sup_{s \in \eta + \mathrm{i}\mathbb{R}} \left| \frac{\widehat{A}(s) - \widehat{J}_0(s)}{\widehat{J}_0(s)} \right| < \varepsilon$$

where ε is a prescribed tolerance and $\eta > 0$ is a shift to avoid poles
  - This method of approximating J_0 is also used for radiation boundary conditions

Modification of current paradigm - Part V





- Toy model to compare current and modified paradigms:
  - "Field":

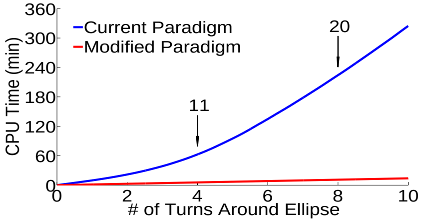
$$F(\mathbf{R},u) = \int_0^u dv \int_{-\pi}^{\pi} d\theta G(\mathbf{R} + (u-v)\mathbf{e}(\theta), v) \ ,$$

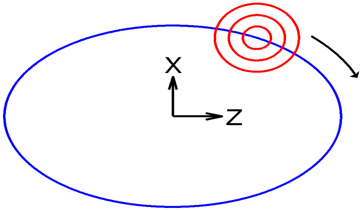
with "source" given by

$$G(\mathbf{R},u) = \exp\left(-\nu|\mathbf{R} - \mathbf{R}_c(u)|^2\right) \ ,$$
$$\mathbf{R}_c(u) = (a\cos(\omega u), b\sin(\omega u)) \ .$$

Source G is essentially a Gaussian moving on an ellipse.

Modification of current paradigm - Part VI





- Toy model (continued)
  - We take $\nu = 5, \omega = 2\pi, a = 1.2, b = 0.8$
  - We calculate $F(\mathbf{R}, n\Delta)$ on $Z \times X$ grid with $64 \cdot 48$ grid points
  - Left figure displays the expected quadratic growth in CPU time for current paradigm using quad2D integrator from Matlab.
  - In modified paradigm the CPU time grows linearly
  - CPU times consistent with flop # and function evaluation #
  - We used $64 \cdot 48$ grid points in $k_Z \cdot k_X$ with maximal $|\mathbf{k}|$-value around 26 so that needed domain of J_0 is $[0, 260]$. We used $N_E = 56$ where relative error (with respect to the envelope) of J_0 on interval $[0, 10^6]$ is ≤ 0.01. Relative error only blows up beyond interval $[0, 10^7]$.

Future paradigm

- Consider sheet bunch or more general bunch
- Do direct time integration of VM system of PDEs
- This eliminates integral over history but requires fields outside bunch
- Thus use radiation boundary conditions to restrict field domain to subset of space between the shielding plates
- For spatial discretization we will begin by investigating Discontinuous Galerkin methods and their implementation in the code HEDGE (Hybrid Easy Discontinuous Galerkin Environment).
- This work will be part of a Ph.D. dissertation project by one of us (D.B.).
- Discontinuous Galerkin method is closely related to Finite Element method