AN APPLICATION OF THE NON-CONFORMING CROUZEIX-RAVIART FINITE ELEMENT METHOD TO SPACE CHARGE CALCULATIONS

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Abstract

The calculation of space charge effects in linear accelerators is an important prerequisite to understand the interaction between charged particles and the surrounding environment. These calculations should be as efficient as possible. In this work we explore the suitability of the Crouzeix-Raviart Finite Element Method for the computation of the self-field of an electron bunch.

INTRODUCTION

Current and future accelerator design requires efficient 3D space charge calculations. One possible approach to Space Charge Calculations is the Particle-in-Cell (PIC) method, especially the Particle-Mesh method which calculates the potential in the rest-frame of the bunch.

This computation usually is done by solving Poisson's equation on the domain Ω, using a charge weighting $\mathsf{f}(x)$:

$$-\Delta\,\mathsf{u}(x) \quad = \quad \mathsf{f}(x), \qquad \forall x \in \Omega.$$

This equation is subject to some boundary conditions:

$$\begin{aligned} \mathsf{u}(x) &= g_D(x), && \forall x \in \partial\Omega_D, \\ \operatorname{grad}\mathsf{u}(x)\cdot n(x) &= g_N(x), && \forall x \in \partial\Omega_N. \end{aligned}$$

These computations should be as efficient as possible.

SPACE CHARGE CALCULATIONS

We are aiming at computing the self-field of the bunch. Denoting with $\mathbf{D}$ the dielectric flux and with ρ the charge density we are estimating a solution to Gauss' law:

$$\operatorname{div}\mathbf{D} = \rho.$$

Usually there are infinitely many solutions to that equation, as in fact a very large subspace of all vectorial functions on the domain fulfils the equation. One can add any divergence-free field (for example a rotational field) to a known solution without changing the divergence, therefore recovering additional solutions to the field equation.

For the moment we are only interested in curl-free solutions of Gauss' law, so we will only try to estimate fields $\mathbf{\Psi}(x)$ which are gradients of a scalar potential $\mathsf{u}(x)$, as: $\mathbf{\Psi}(x) = -\operatorname{grad}\mathsf{u}(x)$, so our equations become:

$$\begin{aligned} \operatorname{grad}\mathsf{u}(x) + \mathbf{\Psi}(x) &= \mathbf{0} && \forall x \in \Omega, \\ -\operatorname{div}\boldsymbol{\varepsilon}(x)\,\mathbf{\Psi}(x) &= \rho(x) && \forall x \in \Omega. \end{aligned}$$

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Removing the auxiliary vector function $\mathbf{\Psi}(x)$ this usually gets shortened to the following equation:

$$-\operatorname{div}\boldsymbol{\varepsilon}(x)\operatorname{grad}\mathsf{u}(x) = \rho(x) \qquad \forall x \in \Omega.$$

If the permittivity tensor $\boldsymbol{\varepsilon}(x)$ isotropic and can be replaced by a divergence free scalar function $\varepsilon(x)$ this becomes:

$$-\Delta\mathsf{u}(x) = \varepsilon(x)^{-1}\rho(x) \qquad \forall x \in \Omega.$$

Our currently used numerical scheme [5] - solving Poissons equation $-\Delta\mathsf{u}(x) = \rho(x)/\varepsilon_0$ in vacuum using a finite difference scheme - seems to less than optimal for estimating the electric field.

We are loosing one order of convergence ($O(h^2) \rightarrow O(h^1)$) by the numerically computation of the electric field from the potential u (even if using the exact derivative on the underlying function space).

The discretized solution u_h on an equidistant structured mesh approximates the solution u with an order $O(h^2)$:

$$\mathsf{u}_h(x) = \mathsf{u}(x) + O(h^2).$$

The gradient $\mathbf{\Psi}$ (which corresponds to our accelerating field) will than be approximated with an order of $O(h^1)$:

$$\mathbf{\Psi}_h(x) = \mathbf{\Psi}(x) + O(h^1).$$

As we are mainly interested in the electric field we would like to approximate it with the same order of accuracy as the potential.

So we want to discretize and solve for the vector field $\mathbf{\Psi}$ directly. The discretization used has to be curl-free and should somehow allow for a reasonable definition of the divergence of the field (e.g. be conformal).

Raviart-Thomas Mixed Finite Elements

One suitable ansatz-space is the lowest order Raviart-Thomas space $\mathbf{RT}_0$ whose linear vector functions have following element-wise linear expression:

$$\mathbf{\Psi}_h(\mathbf{x}) \quad = \quad \mathbf{a}_k + b_k\mathbf{x},$$

where $\mathbf{x}$ is in the element T_k of the triangulation $\mathbf{T}$ of $\mathbf{\Omega}$.

For the discretisation to be conformal the normal components of the field have to be continuous at every interface (edges in 2D or faces in 3D).

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To include this continuity constraint in the construction of the finite element space, $\mathbf{RT}_0$ usually is represented by an interface-based discretization using following definition:

$$\psi_{E_j}(\mathbf{x}) = \sigma_j \frac{|E_j|}{2|T_k|}(\mathbf{x} - \mathbf{P}_j).$$

Where $|T_k|$ is the area/volume of the simplex T_k, $|E_j|$ is the length/area of the edge/face E_j, σ_j indicates the orientation of E_j and $\mathbf{P}_j$ is the vertex opposite to E_j.

Mixed and Hybrid Formulation

We are now using the canonical Galerkin-approach for Mixed Finite Elements to compute approximate solutions for the field $\mathbf{\Psi}_h$ and the potential u_h:

$$\begin{aligned} \int_\Omega \boldsymbol{\tau} \cdot \mathbf{\Psi}_h + \int_\Omega \boldsymbol{\tau}\, \varepsilon \,\mathrm{grad}\, u_h &= 0 \quad \forall \boldsymbol{\tau} \in \mathbf{RT}_0, \\ \int_\Omega v \,\mathrm{div}\, \mathbf{\Psi}_h &= \int_\Omega v\, f \quad \forall v \in \mathbf{P}_1^{-1}. \end{aligned}$$

To later remove the flux variable from the system, one can relax the continuity requirement on the ansatz-space and use the flux $\tilde{\mathbf{\Psi}}_h$ from the space $\mathbf{RT}_0^{-1}$ of piecewise linear vector and discontinuous vector functions.

One could then enforce the continuity of the normal component of the flux on the interfaces by the use of piecewise discontinuous Lagrange multipliers $\lambda_h \in \mathbf{M}_1^{-1}$, leading to following system of equations:

$$\begin{aligned} \int_\Omega \tilde{\boldsymbol{\tau}} \cdot \tilde{\mathbf{\Psi}}_h + \int_\Omega \tilde{\boldsymbol{\tau}}\, \varepsilon \,\mathrm{grad}\, u_h + \int_{\delta\Omega} \lambda_h\, \mathbf{n}_T \cdot \tilde{\boldsymbol{\tau}} &= 0, \\ \int_\Omega v \,\mathrm{div}\, \tilde{\mathbf{\Psi}}_h &= \int_\Omega v\, f, \\ \int_{\delta\Omega} \mu\, \mathbf{n}_T \cdot \tilde{\mathbf{\Psi}}_h &= 0. \end{aligned}$$

for all $\tilde{\boldsymbol{\tau}}$, v and μ in $\mathbf{RT}_0^{-1}$, $\mathbf{P}_1^{-1}$ and $\mathbf{M}_1^{-1}$ respectively.

This is equivalent to a system of linear equations such as:

$$\begin{pmatrix} \mathbf{A} & \mathbf{B} & \mathbf{C} \\ \mathbf{B}^T & & \\ \mathbf{C}^T & & \end{pmatrix} \begin{pmatrix} \tilde{\mathbf{\Psi}}_h \\ u_h \\ \lambda_h \end{pmatrix} = \begin{pmatrix} 0 \\ f_h \\ 0 \end{pmatrix}.$$

Because $\mathbf{A}$ is block-diagonal it is element-wise invertible, the local $\tilde{\mathbf{\Psi}}_h$ can easily be computed by:

$$\tilde{\mathbf{\Psi}}_h = -\mathbf{A}^{-1}(\mathbf{B}\, u_h + \mathbf{C}\, \lambda_h).$$

Using block Gauss elimination this leads to the following system of linear equations:

$$\begin{pmatrix} \mathbf{B}^T\mathbf{A}^{-1}\mathbf{B} & \mathbf{B}^T\mathbf{A}^{-1}\mathbf{C} \\ \mathbf{C}^T\mathbf{A}^{-1}\mathbf{B} & \mathbf{C}^T\mathbf{A}^{-1}\mathbf{C} \end{pmatrix} \begin{pmatrix} u_h \\ \lambda_h \end{pmatrix} = \begin{pmatrix} -f_h \\ 0 \end{pmatrix}.$$

This method is called static condensation. Also eliminating the u_h using a Schur complement one arrives at the Crouzeix-Raviart Finite Element Method, which can also be derived differently.

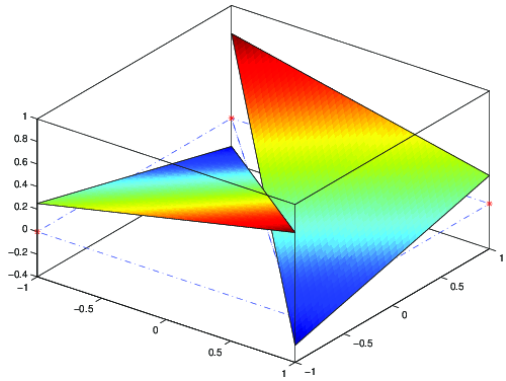

Figure 1: The ansatz-functions are only continuous at the midpoints of interfaces

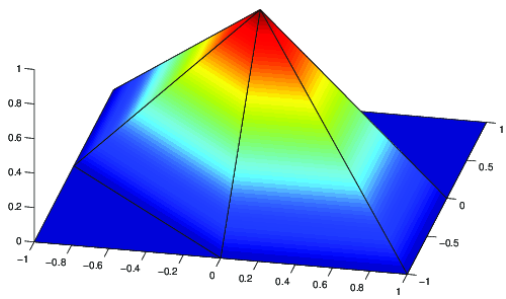

Figure 2: The space of continuous $\mathbf{P}_1$ is contained in $\mathbf{P}_1^{\mathsf{NC}}$.

Crouzeix-Raviart Non-conformal FEM

In [1] Marini suggested to directly use the locally $\mathbf{P}_1$ but nonconforming finite element spaces $\mathbf{P}_1^{\mathsf{NC}}$, these are also called Crouzeix-Raviart or loof finite element spaces. (This approach can also be found in [2])

These finite elements have their degrees of freedom allocated at the barycenters of their interfaces, rather than at their vertices. The function space $\mathbf{P}_1^{\mathsf{NC}}$ actually contains the contains the space $\mathbf{P}_1$ of Lagrange finite elements, so it can at least represent the continuous solutions from nodal $\mathbf{P}_1$ discretizations, but it is larger.

The direct way to arrive at the Crouzeix-Raviart Finite Element Method is to apply the usual Galerkin approach to the nonconforming ansatz space $\mathbf{P}_1^{\mathsf{NC}}$ directly:

$$\sum_{T_k \in \mathbf{T}} \int_{T_k} \varepsilon \,\mathrm{grad}_h\, \mathsf{u}_h \cdot \mathrm{grad}_h\, v = \int_\Omega f_h v \quad \forall v \in \mathbf{P}_1^{\mathsf{NC}}.$$

With decreasing mesh size h the numerical solution u_h converges to u with $O(h^2)$. More interestingly a special post-processing can recover a linear flux $\mathbf{\Psi}_h(x)$ of second order accuracy $O(h^2)$ from $\mathsf{u}_h(x)$ by locally choosing:

$$\mathbf{\Psi}_h(x) = \varepsilon \,\mathrm{grad}_h\, \mathsf{u}_h - f_h\, (\mathbf{x} - \mathbf{x}_{T_k})/n$$

on the element T_k. (with n denoting the dimension of the problem setting and $\mathbf{x}_{T_k}$ the barycenter of the simplex T_k)

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Table 1: Tabulated convergence of successive refinements of the square domain $[0,1]\times[0,1]$; $\|e_{\mathsf{u}_h}\|_2$ and $\|e_{\mathsf{u}_h}\|_\infty$ are the L_2 and the maximum error of the potential u_h, while $\|e_{\mathbf{\Psi}_h}\|_\infty$ indicates the maximum error of the approximated gradient $\mathbf{\Psi}_h$ at interface midpoints.

K	t(sec)	$\|e_{\mathsf{u}_h}\|_2$	$\|e_{\mathsf{u}_h}\|_\infty$	$\|e_{\mathbf{\Psi}_h}\|_\infty$
40	0.002	6.20e-2	1.20e-1	2.85e+0
176	0.004	1.49e-2	3.69e-2	1.28e+0
736	0.009	3.70e-3	9.59e-3	3.65e-1
3008	0.035	9.24e-4	2.40e-3	9.47e-2
12160	0.204	2.31e-4	6.01e-4	2.39e-2
48896	1.433	5.77e-5	1.50e-4	5.97e-3

Table 2: Tabulated convergence of successive refinements of the cube $[0,1]\times[0,1]\times[0,1]$; $\|e_{\mathsf{u}_h}\|_2$, $\|e_{\mathsf{u}_h}\|_\infty$ and $\|e_{\mathbf{\Psi}_h}\|_\infty$ retain the meaning indicated in Table 1.

K	t(sec)	$\|e_{\mathsf{u}_h}\|_2$	$\|e_{\mathsf{u}_h}\|_\infty$	$\|e_{\mathbf{\Psi}_h}\|_\infty$
6	0.002	1.42e+0	9.74e-1	1.44e+1
72	0.002	7.14e-1	9.20e-1	1.32e+1
672	0.006	1.49e-1	3.20e-1	6.87e+0
5760	0.044	4.02e-2	1.13e-1	2.93e+0
47616	0.597	1.07e-2	3.21e-2	8.63e-1
387072	9.373	2.74e-3	8.58e-3	2.23e-1

RESULTS

For convergence studies we have implemented Crouzeix-Raviart Finite Elements in MATLAB [6] for two and three dimensional simplical meshes.

For benchmarking the robustness and for accessing the efficiency of this approach we are solving:

$$\begin{aligned} -\Delta \mathsf{u}(x) &= 3\pi^2\, sin(\pi x_1)\, sin(\pi x_2)\, sin(\pi x_3) \text{ in 3D,} \\ -\Delta \mathsf{u}(x) &= 2\pi^2\, sin(\pi x_1)\, sin(\pi x_2) \text{ in 2D.} \end{aligned}$$

The analytic solutions for the scalar potential u is given by:

$$\begin{aligned} \mathsf{u}(x) &= sin(\pi x_1)\, sin(\pi x_2)\, sin(\pi x_3) \quad \text{in 3D} \\ \mathsf{u}(x) &= sin(\pi x_1)\, sin(\pi x_2) \quad \text{in 2D respectively.} \end{aligned}$$

The convergence of the solution for successively refined meshes (halving the minimum element diameter in each step) is tabulated for two dimensions in table 1 and for three dimensions in table 2.

The convergence of the potential shows the expected behaviour (order $O(h^2)$ implying a reduction of the error by a factor of 4 when the step-size is halved).

The error in the approximated field distribution seems to be dominated by the error at the boundary (especially the corners of the domain) first - only approaching order $O(h^2)$ on highly refined grids.

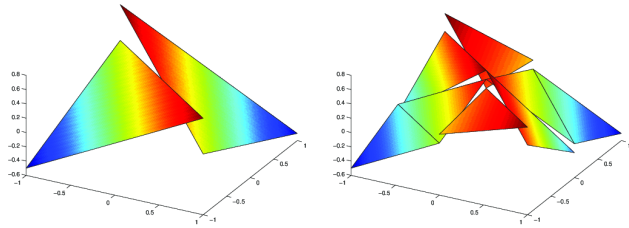

Figure 3: Coarse grid function is not contained in fine grid

CONCLUSIONS

Though in both cases the computation time using the conjugate gradient algorithm could be reduced by a factor of 2 by using SSOR as a preconditioner for our current applications and the accuracy sought the computational cost seems to be prohibitive.

The algorithm still does not have the optimal complexity. Besides using an efficient preconditioner we want to explore the use of geometric multigrid for Crouzeix Raviart finite elements.

Using the right prolongation and restriction operators is not completely straight-forward for the finite element spaces involved as the successively refined function spaces are not nested (see Figure 3). Exploring the approaches in [4] and geometric multigrid as described in [3] seems to be most promising at the moment.

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