Dynamical Solver for Coulomb Explosions in a Magnetic Field

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Abstract

A Coulomb explosion is a micro-plasma phenomenon in which an ionized cluster (or droplet) undergoes rapid expansion due to electrostatic repulsion between the ions. This is a single species plasma, with possible application for tabletop fusion neutron source. An interesting dynamic arises when such rapid expansion happens in a magnetic field. In this case, a rotation of the charge distribution occurs, and a "restoring force" appears, limiting the outer radius of the expansion in the direction perpendicular to the magnetic field.

In this project, I'll solve the dynamics of the Coulomb explosion of the single ion species. I'll use a fluid approximation, which is formulated as set of PDEs in time and 2 spatial dimensions.

1 Model Equations

The set of equations I am planning on solving is:

$$\begin{split} \nabla^2 \varphi &= -\frac{en}{\varepsilon} \\ \vec{E} &= -\nabla \varphi \\ \frac{\partial n}{\partial t} + \nabla \cdot (\vec{v}n) &= 0 \\ mn \frac{\partial \vec{v}}{\partial t} &= -mn \vec{v} \cdot \nabla \vec{v} - \nabla P + Zen \left(\vec{E} + \vec{v} \times \vec{B} \right) \end{split}$$

With P being a constant for now, $\vec{B} = B_0 \hat{z} = Cosnt.$, with the intention of implementing the next Braginskii equation for the pressure later.

The boundary conditions are perfectly conducting walls, $\varphi=0$, and no particle flux through them $\vec{v}\cdot\hat{n}=0$ Initial conditions will be $\vec{v}=0$ and $n=n_0\Theta\left(1-\frac{x^2}{R_0^2}-\frac{y^2}{R_0^2}\right)$ with Θ being the Heaviside function.

2 FE Solver for Electric Potential

One of the required steps in solving an electrostatic plasma approximation is an electric field integrator. The purpose of this module is to produce an electric potential using boundary conditions and the space charge density in the domain. For this purpose, and because of the general usefulness of the tool, the finite element method was chosen, with quadratic elements involving eight nodes on the element boundary.

The first sub-module in this section is a mesher, used to define a grid of $N_col x N_row$ elements, define the nodes and prepares the data for the solver.

2.1 Problem formulation

In a finite element solver, we use continuous Galerkin method to approximate the solution to a (partial) differential equation. The partial differential equation implemented in this code is the Poisson equation, written in the form

$$-\nabla \varepsilon(\vec{r}) \nabla u = f(\vec{r}), \qquad \vec{r} \epsilon \Omega$$
$$\sigma u + \beta \nabla u \cdot \hat{n} = q \qquad \vec{r} \epsilon \partial \Omega$$

with ε generally being a second-order tensor.

For this project, $\varepsilon = 1$, a scalar, $f(\vec{r}) = \frac{Zen_i}{\varepsilon}$, with Z = 1 for hydrogen isotopes, e being the elementary charge, and ε beign the vacuum permittivity.

Here, we will solve Cartesian-coordinate domain, thus the ∇ operators break down into $\nabla = \hat{x} \frac{\partial}{\partial x} + \hat{y} \frac{\partial}{\partial y}$ The Residual R within the domain Ω is the difference between the approxi-

The Residual R within the domain Ω is the difference between the approximate solution \bar{u} to the exact solution, u.

$$R = -\left(\frac{\partial}{\partial x}\varepsilon_x \frac{\partial \bar{u}}{\partial x} + \frac{\partial}{\partial y}\varepsilon_y \frac{\partial \bar{u}}{\partial y}\right) - f$$

The approximate solution is assumed to be

$$\bar{u} = c_i N_i$$

with c_j being scalar coefficients and N_j orthonormal functions in the domain.

We will minimize the internal product of the residual with the basis functions N_i :

$$\langle R, N_i \rangle = \int_{\Omega} \left(-N_i \nabla \varepsilon(\vec{r}) \nabla c_j N_j - f N_i \right) dx dy$$
$$\langle R, N_i \rangle = -\int_{\Omega} f N_i dx dy - \int_{\Omega} N_i \nabla \varepsilon(\vec{r}) \nabla c_j N_j dx dy$$

Partially integrating the last integral:

$$\int_{\Omega} N_{i} \nabla \varepsilon(\vec{r}) \nabla N_{j} dx dy = \int_{\partial \Omega} \left(\varepsilon(\vec{r}) \nabla N_{j} \right) \cdot \hat{n} N_{i} ds - \int_{\Omega} \nabla N_{i} \cdot \left(\varepsilon(\vec{r}) \nabla N_{j} \right) dx dy$$

The residual on the domain boundary $\partial\Omega$ is the difference between the prescribed boundary conditions to the boundary condition the approximate solution satisfies:

$$r = \sigma c_j N_j + \beta \nabla c_j N_j \cdot \hat{n} - q$$

Integrating the boundary residual and adding the domain residual integral:

$$\langle R, N_i \rangle_{\Omega + \partial \Omega} = c_j \int_{\Omega} \nabla N_i \cdot (\varepsilon(\vec{r}) \nabla N_j) \, dx dy - c_j \int_{\partial \Omega} (\varepsilon(\vec{r}) \nabla N_j) \cdot \hat{n} N_i ds$$

$$+ c_j \int_{\partial \Omega} \sigma N_j N_i ds + c_j \int_{\partial \Omega} (\beta \nabla N_j \cdot \hat{n}) \, N_i ds - \int_{\Omega} f N_i dx dy - \int_{\partial \Omega} q N_i ds$$

This formulation is called the weak formulation for the Galerkin method. An inspection shows that all but the two last integrals would produce matrices multiplying the coefficient vector, and the two last integrals would produce inhomogeneous terms.

The equation left to solve is:

$$\left(k_{ij}^{\varepsilon} + k_{ij}^{\beta - \varepsilon}\right)c_j = F_i$$

With the stiffness matrices values determined by the basis functions N_j .

In our case, we will choose $\beta = \varepsilon$, so $k_{ij}^{\beta-\varepsilon} = 0$. Let us calculate the values k_{ij}^{ε} , assuming $\varepsilon = Const$. and for the domain $x, y \in [-1, 1] \otimes [-1, 1].$

The traditional basis functions are Lagrange polynomials, each with the value 1 at its node, and 0 at all other nodes. This way, the value of the potential at any node is equal to the coefficient of the node.

The basis function for the domain are:

$$\begin{array}{c|c} N_1 & 1/4\xi(\xi-1)\eta(\eta-1) \\ N_2 & 1/4\xi(1+\xi)\eta(\eta-1) \\ N_3 & 1/4\xi(1+\xi)\eta(\eta+1) \\ N_4 & 1/4\xi(\xi-1)\eta(\eta+1) \\ N_5 & 1/2\eta(\eta-1)(1-\xi^2) \\ N_6 & 1/2\xi(1+\xi)(1-\eta^2) \\ N_7 & 1/2\eta(1+\eta)(1-\xi^2) \\ N_8 & 1/2\xi(\xi-1)(1-\eta^2) \\ N_9 & (1-\xi^2)(1-\eta^2) \end{array}$$

And their gradients are:

∇N	$\hat{\xi}$	$\hat{\eta}$
∇N_1	$1/4(2\xi - 1)\eta(\eta - 1)$	$1/4\xi(\xi-1)(2\eta-1)$
∇N_2	$1/4(1+2\xi)\eta(\eta-1)$	$1/4\xi(1+\xi)(2\eta-1)$
∇N_3	$1/4(1+2\xi)\eta(\eta+1)$	$1/4\xi(1+\xi)(2\eta+1)$
∇N_4	$1/4(2\xi - 1)\eta(\eta + 1)$	$1/4\xi(\xi-1)(2\eta+1)$
∇N_5	$-\xi\eta(\eta-1)$	$1/2(2\eta-1)(1-\xi^2)$
∇N_6	$1/2(1+2\xi)(1-\eta^2)$	$-\eta \xi (1+\xi)$
∇N_7	$-\xi\eta(1+\eta)$	$1/2(1+2\eta)(1-\xi^2)$
∇N_8	$(\xi - 1/2)(1 - \eta^2)$	$\xi \eta (1-\xi)$
∇N_9	$-2\xi(1-\eta^2)$	$-2\eta(1-\xi^2)$

2.1.1 Calculating k_{ij}^{ε}

The stiffness matrix elements $k_{0ij}^{\varepsilon}=\int_{\Omega}\nabla N_i\cdot\nabla N_jdxdy$ for a rectangular 2x2 grid would be:

$$k^{\varepsilon} = \begin{bmatrix} \frac{28}{45} & -\frac{1}{30} & -\frac{1}{45} & -\frac{1}{30} & -\frac{1}{5} & \frac{1}{9} & \frac{1}{9} & -\frac{1}{5} & -\frac{16}{45} \\ -\frac{1}{30} & \frac{28}{45} & -\frac{1}{30} & -\frac{1}{45} & -\frac{1}{5} & -\frac{1}{5} & \frac{1}{9} & \frac{1}{9} & -\frac{16}{45} \\ -\frac{1}{45} & -\frac{1}{30} & \frac{28}{45} & -\frac{1}{30} & \frac{1}{9} & -\frac{1}{5} & -\frac{1}{5} & \frac{1}{9} & -\frac{16}{45} \\ -\frac{1}{30} & -\frac{1}{45} & -\frac{1}{30} & \frac{28}{45} & \frac{1}{9} & \frac{1}{9} & -\frac{1}{5} & -\frac{1}{5} & -\frac{16}{45} \\ -\frac{1}{5} & -\frac{1}{5} & \frac{1}{9} & \frac{1}{9} & \frac{88}{45} & -\frac{16}{45} & 0 & -\frac{16}{45} & -\frac{16}{15} \\ \frac{1}{9} & -\frac{1}{5} & -\frac{1}{5} & \frac{1}{9} & -\frac{1}{6} & \frac{88}{45} & -\frac{16}{45} & 0 & -\frac{16}{15} \\ -\frac{1}{5} & \frac{1}{9} & \frac{1}{9} & -\frac{1}{5} & -\frac{16}{45} & 0 & -\frac{16}{45} & \frac{88}{45} & -\frac{16}{15} \\ -\frac{16}{45} & -\frac{16}{45} & -\frac{16}{45} & -\frac{16}{45} & -\frac{16}{15} & -\frac{16}{15} & -\frac{16}{15} & -\frac{16}{15} \\ -\frac{16}{45} & -\frac{16}{45} & -\frac{16}{45} & -\frac{16}{45} & -\frac{16}{15} & -\frac{16}{15} & -\frac{16}{15} & -\frac{16}{15} & -\frac{16}{15} \\ -\frac{16}{45} & -\frac{16}{45} & -\frac{16}{45} & -\frac{16}{45} & -\frac{16}{15} & -\frac{16}{15} & -\frac{16}{15} & -\frac{16}{15} & -\frac{16}{15} \\ -\frac{16}{45} & -\frac{16}{45} & -\frac{16}{45} & -\frac{16}{45} & -\frac{16}{15} & -\frac{16}{15} & -\frac{16}{15} & -\frac{16}{15} & -\frac{16}{15} \\ -\frac{16}{45} & -\frac{16}{45} & -\frac{16}{45} & -\frac{16}{45} & -\frac{16}{15} & -\frac{16}{15} & -\frac{16}{15} & -\frac{16}{15} \\ -\frac{16}{45} & -\frac{16}{45} & -\frac{16}{45} & -\frac{16}{45} & -\frac{16}{15} & -\frac{16}{15} & -\frac{16}{15} & -\frac{16}{15} \\ -\frac{16}{45} & -\frac{16}{45} & -\frac{16}{45} & -\frac{16}{45} & -\frac{16}{15} & -\frac{16}{15} & -\frac{16}{15} & -\frac{16}{15} \\ -\frac{16}{45} & -\frac{16}{45} & -\frac{16}{45} & -\frac{16}{45} & -\frac{16}{15} & -\frac{16}{15} & -\frac{16}{15} \\ -\frac{16}{45} & -\frac{16}{45} & -\frac{16}{45} & -\frac{16}{45} & -\frac{16}{15} & -\frac{16}{15} & -\frac{16}{15} \\ -\frac{16}{45} & -\frac{16}{45} & -\frac{16}{45} & -\frac{16}{45} & -\frac{16}{15} & -\frac{16}{15} & -\frac{16}{15} \\ -\frac{16}{45} & -\frac{16}{45} & -\frac{16}{45} & -\frac{16}{45} & -\frac{16}{15} & -\frac{16}{15} & -\frac{16}{15} \\ -\frac{16}{45} & -\frac{16}{45} & -\frac{16}{45} & -\frac{16}{45} & -\frac{16}{45} & -\frac{16}{45} & -\frac{16}{45} \\ -\frac{16}{45} & -\frac{16}{45} & -\frac{16}{45} & -\frac{16}{45} & -\frac{16}{45} & -\frac{16}{45} \\ -\frac{16}{45} & -\frac{16}{45} & -\frac{16}{$$

But this is not the case for a deformed grid. For a general grid, a change of variables should be made, with $x,y=XY\cdot\vec{N}(\xi,\eta)$ where \vec{N} is a column vector of the basis functions, and XY is a (2,9) matrix composed of column vectors $\begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix}$ of the vertices of the mapping.

Because the permittivity is taken to be a constant, the exact k_{ij}^{ε} matrix elements are:

$$\begin{split} k_{ij}^{\varepsilon} &= \int\limits_{-1}^{1} \int\limits_{-1}^{1} \left\{ \frac{\partial N_{i}}{\partial \xi} \frac{\partial N_{j}}{\partial \xi} \left[\left(\frac{\partial \xi}{\partial x} \right)^{2} + \left(\frac{\partial \xi}{\partial y} \right)^{2} \right] + \frac{\partial N_{i}}{\partial \eta} \frac{\partial N_{j}}{\partial \eta} \left[\left(\frac{\partial \eta}{\partial x} \right)^{2} + \left(\frac{\partial \eta}{\partial y} \right)^{2} \right] \\ &+ \left(\frac{\partial N_{i}}{\partial \xi} \frac{\partial N_{j}}{\partial \eta} + \frac{\partial N_{i}}{\partial \eta} \frac{\partial N_{j}}{\partial \xi} \right) \left(\frac{\partial \xi}{\partial x} \frac{\partial \eta}{\partial x} + \frac{\partial \xi}{\partial y} \frac{\partial \eta}{\partial y} \right) \left\{ \frac{\partial N_{n}}{\partial \xi} \frac{\partial N_{m}}{\partial \eta} \left(X_{n} Y_{m} - Y_{n} X_{m} \right) d\xi d\eta \right\} \end{split}$$

According to the inverse function theorem $\frac{\partial \xi}{\partial x} = \frac{1}{|J|} \frac{\partial y}{\partial \eta} = \frac{1}{|J|} Y_k \frac{\partial N_k}{\partial \eta}, \ \frac{\partial \xi}{\partial y} = -\frac{1}{|J|} \frac{\partial x}{\partial \eta} = -\frac{1}{|J|} X_k \frac{\partial N_k}{\partial \eta}, \ \frac{\partial \eta}{\partial x} = -\frac{1}{|J|} \frac{\partial y}{\partial \xi} = -\frac{1}{|J|} Y_k \frac{\partial N_k}{\partial \xi}, \text{ and } \frac{\partial \eta}{\partial y} = \frac{1}{|J|} \frac{\partial x}{\partial \xi} = \frac{1}{|J|} X_k \frac{\partial N_k}{\partial \xi},$ so the matrix elements in terms of known functions are:

$$\begin{split} k_{ij}^{\varepsilon} &= \int\limits_{-1}^{1} \int\limits_{-1}^{1} \left\{ \frac{\partial N_{i}}{\partial \xi} \frac{\partial N_{j}}{\partial \xi} \frac{\partial N_{n}}{\partial \eta} \frac{\partial N_{m}}{\partial \eta} + \frac{\partial N_{i}}{\partial \eta} \frac{\partial N_{j}}{\partial \eta} \frac{\partial N_{n}}{\partial \xi} \frac{\partial N_{m}}{\partial \xi} \right. \\ & \left. - \left(\frac{\partial N_{i}}{\partial \xi} \frac{\partial N_{j}}{\partial \eta} + \frac{\partial N_{i}}{\partial \eta} \frac{\partial N_{j}}{\partial \xi} \right) \frac{\partial N_{n}}{\partial \xi} \frac{\partial N_{m}}{\partial \eta} \right\} \\ & \left. \frac{Y_{n} Y_{m} + X_{n} X_{m}}{\frac{\partial N_{n}}{\partial \xi} \frac{\partial N_{m}}{\partial \eta} \left(X_{a} Y_{b} - Y_{a} X_{b} \right)} d\xi d\eta \right. \end{split}$$

Because there is no guarantee the division of the polynomial in the curly brackets by the polynomial in the denominator leave no remainder, evaluating this integral should be done numerically.

The polynomial in the curly brackets is of degree 6 in both ξ and η , and the polynomial in the denominator is of degree 3 in both ξ and η . In the best case scenario, the resulting integrand would be a 3rd degree polynomial, but it could also have an additive term that is an inverse of a 3rd degree polynomial.

Gauss-Legendre quadrature using n points can exactly find the integral of a polynomial of order 2n-1 in one dimension. For 2 dimensional polynomials with remainder, n=6 is chosen, for increased accuracy in evaluating the remainder, with the option of using n=5 instead.

$$\int_{-1}^{1} \int_{-1}^{1} f(\xi, \eta) d\xi d\eta \approx \sum_{i} \sum_{j} w_{i} w_{j} f(\xi_{i}, \eta_{j})$$

with w_i and x_i from Table 25.4 in Abramowitz and Stegun (1964)

6th order quadrature

x_i	w_i
± 0.238619186083197	0.467913934572691
± 0.661209386466265	0.360761573048139
± 0.932469514203152	0.171324492379170

5th order quadrature

* .		
x_i	w_i	
0	128/225	
$\pm \frac{1}{3} \sqrt{5 - 2\sqrt{\frac{10}{7}}}$	$\frac{322+13\sqrt{70}}{900}$	
$\pm \frac{1}{3}\sqrt{5+2\sqrt{\frac{10}{7}}}$	$\frac{322-13\sqrt{70}}{900}$	

2.1.2 Calculating F_i

Similarly to k_{ij}^{ε} , the force vector elements F_i are the inner product of the basis functions N_i and the charge density divided by the permittivity.

$$F_i = \frac{e}{\varepsilon_0} \int_{\Omega} nN_i dx dy$$

The charge density will be represented by quadratic basis functions as well

$$n = d_j M_j$$

turning the integral into

$$F_{i} = \frac{e}{\varepsilon_{0}} \int_{\Omega} d_{j} N_{i} M_{j} \left| \frac{\partial(x, y)}{\partial(\xi, \eta)} \right| d\xi d\eta$$

$$F_{i} = \frac{e}{\varepsilon_{0}} \int_{-1}^{1} \int_{-1}^{1} N_{i} M_{j} \frac{\partial N_{n}}{\partial \xi} \frac{\partial N_{m}}{\partial \eta} d\xi d\eta \left(X_{n} Y_{m} - Y_{n} X_{m} \right) d_{j} = F_{ij} d_{j}$$

We are left with solving the linear system of equations

$$k_{ij}c_i = F_{ij}d_i$$

with d_i defining the (predetermined) charge distribution.

For now, the FE solver is decoupled from the DG solver, so the charge density is being represented in the FE scheme using the same basis functions $M_k = N_k$, with a separate projection operator to broadcast the Legendre Polynomials into the Lagrange-interpolation polynomials.

3 DG Solver for density

The equation we are intending to solve is

$$\frac{\partial n}{\partial t} + \nabla(\vec{v}n) = 0$$

where, as in the previous section the density is a weighted sum of basis functions $n = d(t)_j M_j$, but in the case of discontinuous Galerkin, each function is defined only in a single element.

We remember that the potential solution c_j corresponds to the value of the solution at each node, and nodes 1-8 are shared between elements.

In the case of discontinuous Galerkin, each element has 9 nodes, each with its own unique charge distribution value.

$$R = \frac{\mathrm{d}d(t)_j}{\mathrm{d}t} M_j + d(t)_j \nabla \cdot (\vec{v} M_j)$$

$$\langle R, M_i \rangle = \int_{\Omega} \left(\frac{\mathrm{d}d(t)_j}{\mathrm{d}t} M_i M_j + d(t)_j M_i \nabla \cdot (\vec{v} M_j) \right) dx dy$$

$$\langle R, M_i \rangle = \frac{\mathrm{d}d(t)_j}{\mathrm{d}t} Mass_{ij} - d(t)_j \int_{\Omega} \vec{v} M_j \cdot \nabla N_i dx dy + d(t)_j \int_{\partial \Omega} M_j M_i \vec{v} \cdot \hat{n} ds$$

Using a 3rd order RK time derivative, the continuity equation becomes:

$$d_j^{(1)} = \left[1 + \Delta t Mass_{ij}^{-1} \left(\int_{\Omega} M_j \vec{v} \cdot \nabla M_i dx dy - \int_{\partial \Omega} M_j M_i \vec{v} \cdot \hat{n} ds \right) \right] d_j^t$$

$$d_j^{(2)} = \frac{3}{4}d_j^t + \frac{1}{4}\left[1 + \Delta t Mass_{ij}^{-1}\left(\int_{\Omega} M_j \vec{v} \cdot \nabla M_i dx dy - \int_{\partial \Omega} M_j M_i \vec{v} \cdot \hat{n} ds\right)\right]d_j^{(1)}$$

$$d_j^{t+1} = \frac{1}{3}d_j^t + \frac{2}{3}d_j^{(2)}\left[1 + \Delta t Mass_{ij}^{-1}\left(\int_{\Omega} M_j \vec{v} \cdot \nabla M_i dx dy - \int_{\partial\Omega} M_j M_i \vec{v} \cdot \hat{n} ds\right)\right]$$

We will use the same basis function form for \vec{v} :

$$\vec{v} = (v_{xk}\hat{x} + v_{yk}\hat{y})\,M_k$$

3.1 Calculating Γ_{ii}^{Ω}

The matrix $\Gamma_{ij}^\Omega=\int_\Omega M_j \vec{v}\cdot \nabla M_i dx dy$ is straightforward to calculate:

$$\begin{split} \Gamma_{ij}^{\Omega} &= \int_{\Omega} M_{j} M_{m} \left(v_{xm} \hat{x} + v_{ym} \hat{y} \right) \cdot \\ & \left[\left(\frac{\partial M_{i}}{\partial \xi} \frac{\partial \xi}{\partial x} + \frac{\partial M_{i}}{\partial \eta} \frac{\partial \eta}{\partial x} \right) \hat{x} + \left(\frac{\partial M_{i}}{\partial \xi} \frac{\partial \xi}{\partial y} + \frac{\partial M_{i}}{\partial \eta} \frac{\partial \eta}{\partial y} \right) \hat{y} \right] \left| \frac{\partial (x,y)}{\partial (\xi,\eta)} \right| d\xi d\eta \\ & = \int_{-1}^{1} \int_{-1}^{1} M_{j} M_{m} \left(\frac{\partial M_{i}}{\partial \xi} \frac{\partial N_{n}}{\partial \eta} - \frac{\partial M_{i}}{\partial \eta} \frac{\partial N_{n}}{\partial \xi} \right) d\xi d\eta (Y_{n} v_{xm} - X_{n} v_{ym}) \end{split}$$

And it is written in the form such that $\bar{\Gamma}_{ijnk}^{\Omega}$ is calculated independently and is multiplied by the node position coordinates and the velocity magnitudes.

3.2 Calculating $\Gamma_{ij}^{\partial\Omega}$

The term $\Gamma_{ij}^{\partial\Omega}=\int_{\partial\Omega}M_jM_i\vec{v}\cdot\hat{n}ds$ however, describes interaction between adjacent elements. The normal vectors \hat{n} at each element edge are:

$$\hat{n}_{0} = \hat{n}\big|_{\eta=-1} = \frac{\frac{\partial y}{\partial \xi}\hat{x} - \frac{\partial x}{\partial \xi}\hat{y}}{\sqrt{\left(\frac{\partial x}{\partial \xi}\right)^{2} + \left(\frac{\partial y}{\partial \xi}\right)^{2}}}$$

$$\hat{n}_{1} = \hat{n}\big|_{\xi=1} = \frac{\frac{\partial y}{\partial \eta}\hat{x} - \frac{\partial x}{\partial \eta}\hat{y}}{\sqrt{\left(\frac{\partial x}{\partial \eta}\right)^{2} + \left(\frac{\partial y}{\partial \eta}\right)^{2}}}$$

$$\hat{n}_{2} = \hat{n}\big|_{\eta=1} = \frac{-\frac{\partial y}{\partial \xi}\hat{x} + \frac{\partial x}{\partial \xi}\hat{y}}{\sqrt{\left(\frac{\partial x}{\partial \xi}\right)^{2} + \left(\frac{\partial y}{\partial \xi}\right)^{2}}}$$

$$\hat{n}_{3} = \hat{n}\big|_{\xi=-1} = \frac{-\frac{\partial y}{\partial \eta}\hat{x} + \frac{\partial x}{\partial \eta}\hat{y}}{\sqrt{\left(\frac{\partial x}{\partial \eta}\right)^{2} + \left(\frac{\partial y}{\partial \eta}\right)^{2}}}$$

$$\begin{split} \Gamma_{ij}^{\partial\Omega} &= \int_{\partial\Omega} M_i M_j \vec{v} \cdot \hat{n} ds = \Gamma_{ij}^{\partial1} + \Gamma_{ij}^{\partial2} + \Gamma_{ij}^{\partial3} + \Gamma_{ij}^{\partial4} \\ & \left[\int_{-1}^{1} M_i M_j M_m \frac{\partial N_n}{\partial \xi} \bigg|_{\eta = -1} d\xi + \int_{-1}^{1} M_i M_j M_m \frac{\partial N_n}{\partial \eta} \bigg|_{\xi = 1} d\eta \right] \\ & - \int_{-1}^{1} M_i M_j M_m \frac{\partial N_n}{\partial \xi} \bigg|_{\eta = 1} d\xi - \int_{-1}^{1} M_i M_j M_m \frac{\partial N_n}{\partial \eta} \bigg|_{\xi = -1} d\eta \right] (Y_n v_{xm} - X_n v_{ym}) \end{split}$$

3.3 Lax-Friedrichs Flux

In order to the fluxes described above are "centered" fluxes. In order to get a more accurate "upwind" fluxes, we will introduce a numerical dissipation.

dissipation = \bar{v}

$$\alpha = |\overline{\vec{v} \cdot \hat{n}}|$$

$$\alpha^{1} = \left| \int_{-1}^{1} M_{m} \frac{\partial N_{n}}{\partial \xi} \right|_{\eta = -1} d\xi \left(Y_{n} v_{xm} - X_{n} v_{ym} \right) \right|$$

$$\alpha^{2} = \left| \int_{-1}^{1} M_{m} \frac{\partial N_{n}}{\partial \eta} \right|_{\xi=1} d\eta \left(Y_{n} v_{xm} - X_{n} v_{ym} \right)$$

$$\alpha^{3} = \left| \int_{-1}^{1} M_{m} \frac{\partial N_{n}}{\partial \xi} \right|_{\eta=1} d\xi \left(Y_{n} v_{xm} - X_{n} v_{ym} \right)$$

$$\alpha^{4} = \left| \int_{-1}^{1} M_{m} \frac{\partial N_{n}}{\partial \eta} \right|_{\xi=-1} d\eta \left(Y_{n} v_{xm} - X_{n} v_{ym} \right)$$

4 Code Structure

4.1 Pre-Processor Module

The pre-processor module handles meshing and matrix assembly for the finiteelement solver. It also partly assembles the geometry-dependent matrices for the discontinuous Galerkin solver.

4.1.1 CheckDetJ(XY,fineness=10)

Before meshing begins, the pre-processor checks the geometry provided for singular values of the determinant. This method receives the geometry definition intended for the NodeArrange method, and checks a fineness x fineness grid of points within for negative |J|.

4.1.2 NodeArrange(N_row,N_col,XY,NodeBeginNum,ElemBeginNum)

This method is a mesher - it arranged nodes within a "macro-element". A "macro-element" is defined by the (2,9) matrix XY, with parametrization x,y= XY· $\vec{N}(\xi,\eta)$. The "macro-element" is divided into N_row rows and N_col columns in ξ and η . As a consequence of this, positioning nodes 5, 7, and 9 to the left of the "macro-element" center would result in a refined mesh in the region to the left of these nodes, and a coarser mesh in the region to the right.

The method returns a list of nodes. Each node is represented by a column, with structure:

```
# node
node x coordinate
node y coordinate
```

and a list of elements, with each element represented by a row, with structure:

```
[# element, # node_1, ..., # node_9]
```

The node numbering is presented in Figure 1.

Additionally, the method returns a connectivity matrix, identifying the element numbers adjacent to each face:

```
[# ele face_1, # ele face_2, # ele face_3, # ele face_4]
```

where face_1 is the face containing node 5, face_2 is the face containing node 6, face_3 is the face containing node 7, and face_4 is the face containing node 8.

4.1.3 assemble Global Mats (Global Element Matrix, Node List, Qorder)

This method assembles the matrices k_{ij} and F_{ij} as described above. It first calculate the matrix for each element, and then adds its values to the global

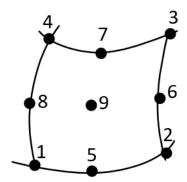


Figure 1: Node numbering within each element

matrices. By default, it calculates 6th order Gaussian quadrature for the elements of k_{ij} , but if Qorder=5, it would calculate a 5th order quadrature instead. It returns GlobalStiffMat, GlobalForceMat.

4.1.4 assembleElementMats(GlobalElementMatrix,NodeList,DGorder)

This method assembles the DG matrices. Since in DG, each element is defined independently, and only the weak form of the fluxes is dealt with, this

4.2 polynomial2d Module, poly Class

The poly class handles 2D polynomial operations. Polynomials are represented as 2D arrays, with coefficients[i,j] representing the coefficient of $y^i x^j$, for the polynomial $p(x,y) = \sum_{i,j} \text{coefficients[i,j]} y^i x^j$. Methods in this class:

4.2.1 __init__(self, coefficients)

Initiates a poly instance, with list, list of lists, or numpy array as the coefficients.

4.2.2 __repr__(self), tex(self), __str__(self)

Returns the canonical string representation of a polynomial in python or tex formats.

4.2.3 __call__(self, x=None,y=None)

Returns the evaluated polynomial as either a 1D polynomial in x or y, if given only a y or x value, or returns the evaluated polynomial as a scalar if given both x and y.

4.2.4 degreex(self), degreey(self)

Returns the degree +1 of the x or y dimension of the polynomial.

4.2.5 degree(self)

Returns the degree +1 of the polynomial.

4.2.6 __add__(self,other), __radd__(self,other), __sub__(self,other)

Performs polynomial addition between two polynomials or between a polynomial and a scalar. Scalars are casted into a 0th degree polynomial, and then added. Subtraction is performed as multiplication by -1 followed by addition.

4.2.7 __mul__(self,other), __rmul__(self,other)

Performs multiplication of polynomials or polynomial and a scalar. Returns a polynomial of degree in x and y being the sums of the degrees in x and y of the constituent polynomials.

4.2.8 dx(self), dy(self)

Performs a derivative operation on a polynomial in x or y. Returns a polynomial with a reduced degree in x or y.

4.2.9 intx(self,ax=None,bx=None), inty(self,ay=None,by=None)

Performs integration in x or y, and returns the integrated polynomial with the constant of integration = 0 - if not given ax, or ay, or the integrated polynomial evaluated at ax or ay - if not given bx or by, or the integral between ax and bx or ay and by.

4.2.10 scalar(self)

Returns the scalar value of a 0th degree polynomial.