Kinetic modeling of thermal quench

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In order to model the thermal quench and the electron distribution function from the first principles, predescribed temporal profiles for the temperature evolution should be abandoned and the related physics included in the kinetic equation. If we are not interested on the current quench, the plasma current can be assumed constant in time admitting a closed set of equations for self-consistent description of the thermal quench. Our model will only investigate the momentum space dynamics, assuming constant profiles accross the plasma and also assumes the plasma to be a straight cylinder. With these approximations, the system of equations becomes simple enough to solve, so that scans over different kinetic mechanisms can be efficiently conducted.

The model we propose includes nonlinear description for the electron-electron collision, linear treatment of electron-ion collisions, and linear source and sink terms. The accelerating electric field is computed from the condition that the plasma current density remains constant. The concept of plasma conductivity is not needed, since the electron-electron collisions are treated nonlinearly and the collisions with ions are included in the model. The spitzer response is thus automatically included.

Since the distribution function is assumed to be elongated along the direction of the electric, especially if the electric exceeds the so-called critical field for runaway generation, we discretize our equations with Finite-Element formulation. This allows efficient use of unstructurized meshes.

I. MODEL EQUATIONS

We assume the plasma to consist of species a, the one we follow from kinetic principles, and of possibly multiple other species b which are assumed to be Maxwellian. The distribution function of species a is assumed to be affected by electric field, Coulomb collisions, by different source and sink terms, e.g., source of cold electrons from ionization of neutrals, or sink of particles mimicking the loss of plasma confinement. The kinetic model for the distribution function of species a is thus described by

$$\frac{\partial f_a}{\partial t} + \frac{e_a \boldsymbol{E}}{m_a} \cdot \frac{\partial f_a}{\partial \boldsymbol{v}} = C_{aa}[f_a, f_a] + C_{ab}[f_a, f_b] + L[f_a] + s, \tag{1}$$

where the Fokker-Planck collision operator for collisions between species a and b is

$$C_{ab}[f_a, f_b] = \left(\frac{e_a^2 e_b^2 \ln \Lambda_{ab}}{m_a^2 \varepsilon_0^2} \right) \frac{\partial}{\partial \boldsymbol{v}} \cdot \left(\frac{m_a}{m_b} \frac{\partial \phi_b}{\partial \boldsymbol{v}} f_a - \frac{\partial^2 \psi_b}{\partial \boldsymbol{v} \partial \boldsymbol{v}} \cdot \frac{\partial f_a}{\partial \boldsymbol{v}} \right). \tag{2}$$

and the Rosenbluth potentials are

$$\phi(\boldsymbol{v}) = -\frac{1}{4\pi} \int f(\boldsymbol{v}') \frac{1}{\mid \boldsymbol{v} - \boldsymbol{v}' \mid} d\boldsymbol{v}', \qquad \psi(\boldsymbol{v}) = -\frac{1}{8\pi} \int f(\boldsymbol{v}') \mid \boldsymbol{v} - \boldsymbol{v}' \mid d\boldsymbol{v}', \tag{3}$$

The operator $L[f_a]$ is assumed be a general linear operator with respect to f_a. The source s is assumed to be independent of f_a. The kinetic equation is coupled to current conservation equation

$$\boldsymbol{E} \cdot \int \boldsymbol{v} \frac{\partial f_a}{\partial t} d\boldsymbol{v} = 0, \tag{4}$$

which then closes our equations. The unknowns in our implicit system are the amplitude of the electric field, E, and the distribution function f_a. Only the magnitude of the electric field is needed, since the distribution has axial symmetry along the direction of the electric field.

A. Normalized equations

Before we proceed any further, it is good practise to swith to dimensionless quantities. We define $\boldsymbol{x} = \boldsymbol{v}/v_0$, where v_0 is a fixed reference velocity. Thus the volume element becomes $d\boldsymbol{v} = v_0^3 d\boldsymbol{x}$ and any velocity space moment becomes $\int \boldsymbol{v}^n f d\boldsymbol{v} = v_0^{3+n} \int \boldsymbol{x}^n f d\boldsymbol{x}$. We also normalize the distribution function and define $F = v_0^3 f/n_0$ so that any physical velocity space moment is given by $\int \boldsymbol{v}^n f d\boldsymbol{v} = n_0 v_0^n \int \boldsymbol{x}^n F d\boldsymbol{x}$. In addition, we define normalized time $\tau = t/t_0$ where

t_0 is a fixed reference time scale. Our equations in the normalized quantities are thus

$$\frac{\partial F_a}{\partial \tau} + \bar{\boldsymbol{E}} \cdot \nabla F_a - \nu_{aa} C[F_a, F_a] - \nu_{ab} C[F_a, F_b] - t_0 L[F_a] - S = 0, \tag{5}$$

$$\bar{\boldsymbol{E}} \cdot \int \boldsymbol{x} \frac{\partial F_a}{\partial \tau} d\boldsymbol{x} = 0 \tag{6}$$

where the normalized dimensionless quantities are

$$\bar{\boldsymbol{E}} = \frac{t_0 e_a}{m v_0} \boldsymbol{E}, \qquad \nu_{ab} = \left(\frac{t_0 n_0 e_a^2 e_b^2 \ln \Lambda_{ab}}{v_0^3 m_a^2 \varepsilon_0^2} \right), \qquad S = \frac{v_0^3 t_0}{n_0} s. \tag{7}$$

The collision operator in the equation is then written simply

$$C[F_a, F_b] = \nabla \cdot \left(\frac{m_a}{m_b} \nabla \Phi_b F_a - \nabla \nabla \Psi_b \cdot \nabla F_a \right) \tag{8}$$

and the Rosenbluth potentials become

$$\Phi(\boldsymbol{x}) = -\frac{1}{4\pi} \int F(\boldsymbol{y}) \frac{1}{\mid \boldsymbol{x} - \boldsymbol{y} \mid} d\boldsymbol{y}, \qquad \Psi(\boldsymbol{x}) = -\frac{1}{8\pi} \int F(\boldsymbol{y}) \mid \boldsymbol{x} - \boldsymbol{y} \mid d\boldsymbol{y}, \tag{9}$$

and satisfy the Poisson equations $\nabla^2 \Phi = F$ and $\nabla^2 \Psi = \Phi$.

II. WEAK FORMULATION WITH BACKWARD EULER STEP

Because the kinetic equation is stiff, the time discretization should be done by backward differentiation. We will use backward Euler, approximating the time derivative of the distribution function at time instance s with the expression $\partial F^s / \partial \tau \approx (F^s - F^{s-1})/\delta\tau$. Further, because we cannot handle infinite domains, the space must be truncated. This requires careful treatment of the Poisson equations, and boundary conditions computed from the Green's function solution.

With that in mind, we multiply the kinetic equation with a test function $F^\star$ and integrate over the computational domain Ω:

$$\int_\Omega F^\star \left(F_a^s - \delta\tau S^s + \delta\tau \bar{\boldsymbol{E}} \cdot \nabla F_a^s + \delta\tau t_0 L[F_a^s] \right) d\boldsymbol{x} + \sum_b \nu_{ab} \delta\tau \int_\Omega \nabla F^\star \cdot \left(\frac{m_a}{m_b} \nabla \Phi_b^s F_a^s - \nabla \nabla \Psi^s \cdot \nabla F^s \right) d\boldsymbol{x}$$
$$- \sum_b \nu_{ab} \delta\tau \int_{\partial\Omega} F^\star \left(F_a^s \frac{m_a}{m_b} \nabla \Phi_b^s - \nabla F_a^s \cdot \nabla \nabla \Psi_b^s \right) \cdot d\boldsymbol{\sigma} = \int_\Omega F^\star F^{s-1} d\boldsymbol{x}. \tag{10}$$

Since the distributions F_b are assumed given, we consider the Poisson equations only for the species a:

$$-\int_\Omega \nabla \Phi_a^s \cdot \nabla \Phi^\star d\boldsymbol{x} + \int_{\partial\Omega} \Phi^\star \nabla \Phi_a^s \cdot d\boldsymbol{\sigma} = \int_\Omega F_a^s \Phi^\star d\boldsymbol{x} \tag{11}$$

$$-\int_\Omega \nabla \Psi_a^s \cdot \nabla \Psi^\star d\boldsymbol{x} + \int_{\partial\Omega} \Psi^\star \nabla \Psi_a^s \cdot d\boldsymbol{\sigma} = \int_\Omega \Phi_a^s \Psi^\star d\boldsymbol{x}. \tag{12}$$

When we truncate the space, the distribution function F_a is assumed to "die off" very fast and to be negligible outside the domain Ω. This allows us to use the truncated definitions for the potential functions and to define Dirichlet conditions for the Poisson equations at the boundary $\partial\Omega$.

To mathematically formulate the weak problems, we assume an n-th order Sobolev space for the test functions $V = \{v \in H^n(\Omega) \mid v(\partial\Omega) = 0\}$ which, together with the conditions that Φ and Ψ are smooth functions, allows us to get rid of the boundary terms in the Poisson equations: A Dirichlet condition is needed to make the potentials unique, the Neumann condition is not needed. The Weak formulation for the first Rosenbluth potential is then

$$-\int_\Omega \nabla \Phi_a^s \cdot \nabla \Phi^\star d\boldsymbol{x} = \int_\Omega F_a^s \Phi^\star d\boldsymbol{x}, \quad \boldsymbol{x} \in \Omega, \quad \forall \Phi^\star \in V \tag{13}$$

$$\Phi_a^s(\boldsymbol{x}) = -\frac{1}{4\pi} \int \frac{F_a^s(\boldsymbol{y})}{\mid \boldsymbol{x} - \boldsymbol{y} \mid} d\boldsymbol{y}, \quad \boldsymbol{x} \in \partial\Omega, \tag{14}$$

and for the second potential we have similarly

$$-\int_\Omega \nabla\Psi_a^s\cdot\nabla\Psi^\star d\boldsymbol{x}=\int_\Omega \Phi_a^s\Psi^\star d\boldsymbol{x},\quad \boldsymbol{x}\in\Omega,\quad \forall\Psi^\star\in V \tag{15}$$

$$\Psi_a^s(\boldsymbol{x})=-\frac{1}{8\pi}\int F_a^s(\boldsymbol{y})\mid \boldsymbol{x}-\boldsymbol{y}\mid d\boldsymbol{y},\quad \boldsymbol{x}\in\partial\Omega. \tag{16}$$

Since we are not imposing Neumann conditions on F_a^s, only the Dirichlet condition, the boundary integral term vanishes in the equation for F_a, and the weak formulation becomes

$$\int_\Omega F^\star\left(F_a^s-\delta\tau S^s-\delta\tau\bar{\boldsymbol{E}}\cdot\nabla F^s+\delta\tau t_0 L[F_a^s]\right)d\boldsymbol{x}+\sum_b\nu_{ab}\delta\tau\int_\Omega\nabla F^\star\cdot\left(\frac{m_a}{m_b}\nabla\Phi_b^sF_a^s-\nabla\nabla\Psi_b^s\cdot\nabla F_a^s\right)d\boldsymbol{x}$$
$$=\int_\Omega F^\star F_a^{s-1}d\boldsymbol{x},\quad \boldsymbol{x}\in\Omega,\quad\forall F^\star\in V. \tag{17}$$

The only complication in our system is the nonlinearity: because the potential functions depend on F_a^s, the weak formulation for F_a^s is not linear. In order to express the kinetic equation completely in terms of the distribution function only, we have to switch to the finite-element presentation, solve the potentials in terms of the degrees of freedom of F_a^s, and put the expressions back into the weak form for the kinetic equation. In the end, we will end up with a bilinear form for the degrees-of-freedom for F_a^s, which is then solved with Newton's method which has a quadratic convergence rate.

A. Degrees-of-freedom representation

We choose our finite-element space to be a set of functions $\{\lambda_i(\boldsymbol{x})\}_{i=1}^N$, and we assume the mesh given. Then we approximate the distribution function to be of the form $F_a^s(\boldsymbol{x})=F_{a,i}^s\lambda_i(\boldsymbol{x})$. If we now compute the Green's function solutions for the potential, we find

$$\Phi_a^s(\boldsymbol{x}_i)=-\frac{1}{4\pi}\int\frac{\lambda_j(\boldsymbol{y})}{\mid\boldsymbol{x}_i-\boldsymbol{y}\mid}d\boldsymbol{y}F_{a,j}^s\equiv G_{ij}^{[\phi]}F_{a,j}^s,\quad \boldsymbol{x}_i\in\partial\Omega, \tag{18}$$

$$\Psi_a^s(\boldsymbol{x}_i)=-\frac{1}{8\pi}\int\lambda_j(\boldsymbol{y})\mid\boldsymbol{x}_i-\boldsymbol{y}\mid d\boldsymbol{y}F_{a,j}^s\equiv G_{ij}^{[\psi]}F_{a,j}^s,\quad \boldsymbol{x}_i\in\partial\Omega. \tag{19}$$

On the other hand, in order to solve the Poisson equations, the potentials must also be expressed as approximations belonging into the finite-element space, i.e., $\Psi_a^s(\boldsymbol{x})=\Psi_{a,i}^s\lambda_i(\boldsymbol{x})$ and $\Phi_a^s(\boldsymbol{x})=\Phi_{a,i}^s\lambda_i(\boldsymbol{x})$. Let's first inspect the equation for the potential Φ_a^s. A straight-forward evaluation of the weak formulation gives us

$$a_{ij}\Phi_{a,j}^s=\lambda_{ij}F_{a,j}^s,\qquad a_{ij}=-\int_\Omega\nabla\lambda_i\cdot\nabla\lambda_j d\boldsymbol{x},\qquad \lambda_{ij}=\int_\Omega\lambda_i\lambda_j d\boldsymbol{x}. \tag{20}$$

Since the basis functions $\lambda_i(\boldsymbol{x})$ are designed in a way that they get the value 1 at the point $\boldsymbol{x}_i$ and are supported only by those mesh elements that have $\boldsymbol{x}_i$ as one of the vertices, and are zero outside the region of support, we have to modify the matrix a_{ij} and λ_{ij} a bit, and our final equations for the first potential become

$$a_{ij}^{[\phi]}\Phi_{a,j}^s=\lambda_{ij}^{[\phi]}F_{a,j}^s,\qquad a_{ij}^{[\phi]}=\lambda_{ij}\left(1-\delta_{iB}\right)+\delta_{iB},\qquad \lambda_{ij}=\int_\Omega\lambda_i\lambda_j d\boldsymbol{x}. \tag{21}$$

III. SPHERICALLY SYMMETRIC COOLING DOWN

The most simple model for the cooling-down process is to assume a zero electric field and a spherically symmetric source of cold particles which drives equilibration of the temperature. The whole kinetic equation will be spherically symmetric, and the weak formulations become quite compact.

In short, we truncate the domain to be a ball limited at radius $\mid\boldsymbol{x}\mid=c$ which then gives

1. the weak formulation for the distribution function: $F^s(c)=0$

$$\int_0^c F^\star(F^s-\Delta\tau S^s)r^2dr+\nu\Delta\tau\int_0^c\partial_rF^\star\partial_r\Phi^sF^sr^2dr-\nu\Delta\tau\int_0^c r^2\partial_rF^\star\partial_{rr}^2\Psi^k\partial_rF^kdv$$
$$=\int_0^c r^2F^\star F^{k-1}dr,\quad\forall F^\star\in V \tag{22}$$

2. the weak formulation for the first Rosenbluht potential:

$$-\int_0^c \partial_r \Phi^s \partial_r \Phi^\star r^2 dr = \int_0^c \Phi^\star F^s, \quad \forall \Phi^\star \in V \tag{23}$$

$$\Phi^s(c) = -\frac{1}{c}\int_0^c F^s r^2 dr. \tag{24}$$

3. the weak formulation for the second Rosenbluth potential:

$$-\int_0^c \partial_r \Psi^s \partial_r \Psi^\star r^2 dr = \int_0^c \Psi^\star \Phi^s, \quad \forall \Psi^\star \in V \tag{25}$$

$$\Psi^s(c) = -\frac{c}{2}\int_0^c F^s r^2 dr - \frac{1}{6c}\int_0^c r^2 F^s r^2 dr. \tag{26}$$

Here we have to keep in mind that the Green's function solutions for the Rosenbluth potentials are truncated to be consistent with the assumption that F vanishes outside the domain

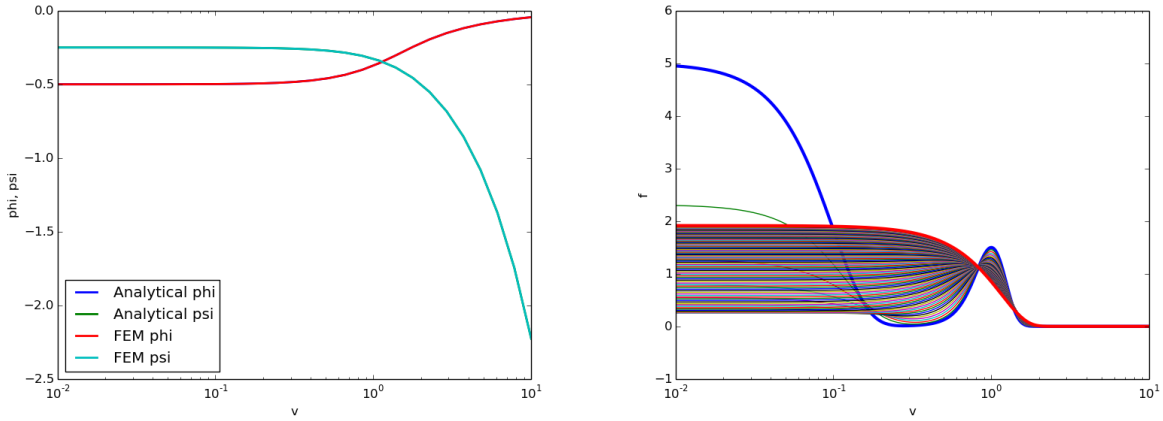

FIG. 1: (left) Comparison of analytical (blue, green) and FEM (red, cyan) solution of the Rosenbluth potentials Φ and Ψ in a Maxwellian plasma. For both potentials the FEM solutions completely overlap with the analytical expressions, and the solutions are numerically stable also at the point $r = 0$. (right) Relaxation of a spherically symmetric non-Maxwellian initial state (thick blue) towards equilibrium (thick red).

The first thing to do is to test the truncated Poisson equations given an analytical distribution function. The most relevant case is to take $F = \exp(-r^2)$, so that the analytical solutions computed from the exact infinite space Greens functions are

$$\Phi = -\frac{\sqrt{\pi}\mathrm{erf}(r)}{4r}, \qquad \Psi = -\frac{2r\exp(-r^2) + \sqrt{\pi}(1+2r^2)\mathrm{erf}(r)}{16r} \tag{27}$$

Using the finite element library FEniCS [1] we solve the truncated potential functions using the weak formulation and compare the result to the analytical solution in Fig. 1. The numerical truncated solution appears to be good, achieving six correct digits at $r = 0$ with second order elements and 30 logarithmically placed mesh points. As a second test, we check the relaxation of nonlinear initial state to equilbrium. Setting $F_0(r) = 1.5\exp\left[-10(r-1)^2\right] + 5\exp\left[-100r^2\right]$, Fig. 1 shows that the backward time differentiation is very robust and would allow very long time steps, as the few first steps demonstrate. Also the density is conserved to machine precision.

Next we add a source term for cold electrons. Using a simple gaussian source with a narrow width and constant rate, we observe the temperature to drop as expected when the total density is increased (see Fig. 2). At the same time the distribution function starts to develop a tail because the collisionality is different for the high-energy particles.

IV. CYLINDRICAL VELOCITY SPACE

Because the electric field in the runaway problem points to the direction parallel to the magnetic field, the cylindrical coordinate with the z-axis directed along the electric field is a natural choice.

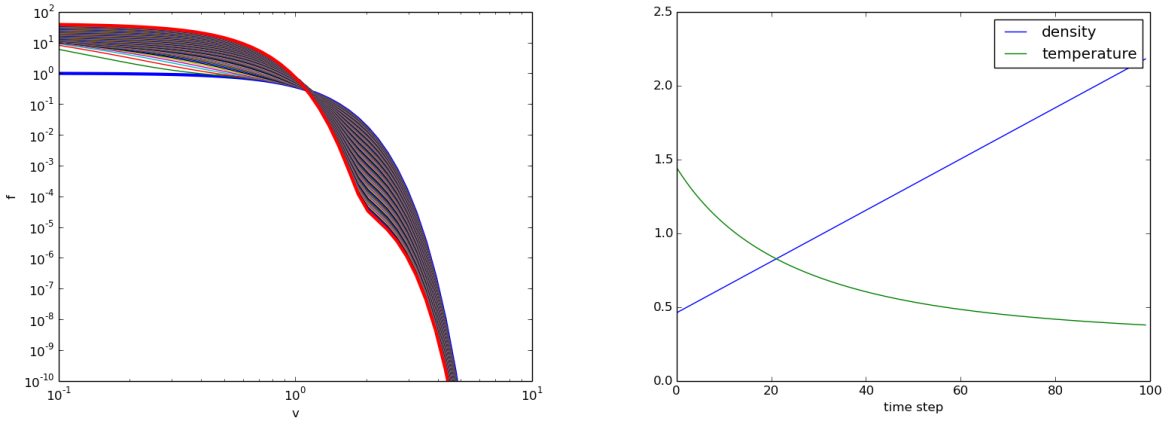

FIG. 2: (Left) Time evolution of the spherically symmetric distribution function due to spherically symmetric source of cold particles. The cold population is increased at constant rate. Thick blue is the initial state and thick red the final time instance. (Right) Temperature and density evolution during the cooling-down.

In cylindrically symmetric case, assuming the electric field to be parallel to the z-axis, we find

1. weak formulation for the distribution function: $F^s(\partial\Omega) = 0$.

$$\iint_\Omega F^\star \left(F^s - \Delta\tau S^s - \Delta\tau \bar{E}^z \partial_z F^s\right) \rho d\rho dz + \nu\Delta\tau \iint_\Omega \left(\partial_\rho F^\star \partial_\rho \Phi^s + \partial_z F^\star \partial_z \Phi^s\right) F^s \rho d\rho dz$$
$$- \nu\Delta\tau \iint_\Omega \left[\partial_\rho F^\star \partial^2_{\rho\rho} \Psi^s \partial_\rho F^s + \partial^2_{\rho z} \Psi^s \left(\partial_\rho F^\star \partial_z F^s + \partial_z F^\star \partial_\rho F^s\right) + \partial_z F^\star \partial^2_{zz} \Psi^s \partial_z F^s\right] \rho d\rho dz$$
$$= \iint_\Omega F^\star F^{s-1} \rho d\rho dz, \quad (\rho, z) \in \Omega, \quad \forall F^\star \in V, \quad (28)$$

2. Weak formulation for the first Rosenbluth potential:

$$-\iint_\Omega \left(\partial_z \Phi \partial_z \Phi^\star + \partial_\rho \Phi \partial_\rho \Phi^\star\right) \rho d\rho dz = \iint F \Phi^\star \rho d\rho dz, \quad (\rho, z) \in \Omega, \quad \forall \Phi^\star \in V \quad (29)$$

$$\Phi(\rho, z) = -\frac{1}{\pi} \iint_\Omega F(\rho', z') \frac{K(k)}{\sqrt{(z - z')^2 + (\rho + \rho')^2}} \rho' d\rho' dz', \quad (\rho, z) \in \partial\Omega, \quad (30)$$

3. Weak formulation for the second Rosenbluth potential:

$$-\iint_\Omega \left(\partial_z \Psi \partial_z \Psi^\star + \partial_\rho \Psi \partial_\rho \Psi^\star\right) \rho d\rho dz = \iint_\Omega \Phi \Psi^\star \rho d\rho dz, \quad (\rho, z) \in \Omega, \quad \forall \Phi^\star \in V \quad (31)$$

$$\Phi(\rho, z) = -\frac{1}{2\pi} \iint_\Omega F(\rho', z') E(k) \sqrt{(z - z')^2 + (\rho + \rho')^2} \rho' d\rho' dz', \quad (\rho, z) \in \partial\Omega, \quad (32)$$

where $k = (4\rho\rho')/[(z - z')^2 + (\rho + \rho')^2]$ and $K(k)$ and $E(k)$ are the complete elliptic integrals of the first and second kind as defined in Mathematica.

Appendix A: Cylindrical coordinates

The cylindrical coordinates $x^i = (\rho, \theta, z)$ relate back to Cartesian coordinates according to

$$x = \rho \sin\theta, \quad y = \rho \sin\theta \tag{A1}$$

so that the metric tensor has non-zero components

$$g_{\rho\rho} = 1, \quad g_{\theta\theta} = \rho^2, \quad g_{zz} = 1, \tag{A2}$$

and the nonzero Christoffel symbols are

$$\Gamma^{\rho}_{\theta\theta} = -\rho \tag{A3}$$

$$\Gamma^{\theta}_{\rho\theta} = \Gamma^{\theta}_{\theta\rho} = 1/\rho. \tag{A4}$$

The distance between two points is given by

$$\mid \boldsymbol{x} - \boldsymbol{x}' \mid = \sqrt{(z-z')^2 + (\rho+\rho')^2}\sqrt{1 - k\cos^2[(\theta-\theta')/2]}, \tag{A5}$$

where

$$k = \frac{4\rho\rho'}{(z-z')^2 + (\rho+\rho')^2} \tag{A6}$$

The angular integrals are thus

$$\int_0^{2\pi} \mid \boldsymbol{x} - \boldsymbol{x}' \mid d\theta' = 4E(k)\sqrt{(z-z')^2 + (\rho+\rho')^2}, \tag{A7}$$

$$\int_0^{2\pi} \mid \boldsymbol{x} - \boldsymbol{x}' \mid^{-1} d\theta' = \frac{4K(k)}{\sqrt{(z-z')^2 + (\rho+\rho')^2}}, \tag{A8}$$

where $K(k)$ and $E(k)$ are the complete elliptic integrals of the first and second kind as defined in Mathematica.

Appendix B: Spherical coordinates

The spherical coordinates $x^i = (x, \xi, \theta)$ relate back to Cartesian coordinates according to

$$x = r\sqrt{1-\xi^2}\cos\theta, \quad y = r\sqrt{1-\xi^2}\sin\theta, \quad z = \xi r, \tag{B1}$$

and the metric is given by

$$g_{rr} = 1, \quad g_{\xi\xi} = \frac{r^2}{1-\xi^2}, \quad g_{\theta\theta} = r^2\left(1-\xi^2\right). \tag{B2}$$

The nonzero Christoffel symbols are

$$\Gamma^{r}_{\xi\xi} = -r/(1-\xi^2) \tag{B3}$$

$$\Gamma^{r}_{\xi\theta} = -r\sqrt{1-\xi^2} \tag{B4}$$

$$\Gamma^{\xi}_{r\xi} = \Gamma^{\xi}_{\xi r} = 1/r \tag{B5}$$

$$\Gamma^{\xi}_{\xi\xi} = \xi/(1-\xi^2) \tag{B6}$$

$$\Gamma^{\xi}_{\theta\theta} = \xi\sqrt{1-\xi^2} \tag{B7}$$

$$\Gamma^{\theta}_{r\theta} = \Gamma^{\theta}_{\theta r} = 1/r \tag{B8}$$

$$\Gamma^{\theta}_{\xi\theta} = \Gamma^{\theta}_{\theta\xi} = -\xi/(1-\xi^2) \tag{B9}$$

[1] Anders Logg and Garth N. Wells. Dolfin: Automated finite element computing. *ACM Trans. Math. Softw.*, 37(2):20:1–20:28, April 2010.