Final Technical Report
Awardee: New York University

DOE Award No. DE-SC0012398
Period of Performance: 07/15/2014 to 10/31/2019
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Introduction

We have been working on the development of high performance numerical solvers for magnetic confinement fusion. The solvers improve on existing codes by drawing from advanced algorithms developed by the applied mathematics community, addressing specific needs stressed by the physicists. Conversely, the particular challenges encountered in fusion applications led us to design solvers with unique features and based on unusual algorithms which triggered interest for further study and development in the applied mathematics community.

A major portion of our research work has concerned the development of integral equation based formulations and solvers for the solution of elliptic partial differential equations describing plasma equilibrium in toroidal configurations. Integral equations have the advantages that they often lead to a reduction in the dimensionality of the problem, and yield high accuracy for derivatives of the solution, which are usually as significant physical quantities as the solution itself. However, special care must be given to the evaluation of the numerical quadratures of integrands which are often singular in order to have a fast solver with the desired accuracy.

A second part of our work has focused on numerical schemes for kinetic equations, which may be hyperbolic or parabolic partial differential equations. A central challenge of kinetic equations is their high dimensionality, requiring efficient representations for the unknowns for computationally tractable simulations. We will discuss new approaches we considered for such simulations.

This document highlights some of the most important numerical schemes we developed, as well as some of my most significant physics results, with a stronger focus on the numerical schemes than the physics results we obtained with these new solvers. The work presented here was done in collaboration with four post-doctoral researchers and a PhD student in our research group, as well as colleagues at the Courant Institute and in the magnetic fusion community.

1 Fast, high order solvers for integrated simulations of magnetically confined plasmas

Modern magnetic confinement fusion experiments have shown that in toroidally axisymmetric devices the transport of particles and energy is mostly mediated by plasma turbulence. This type of transport, often called “anomalous” transport, leads to energy and particle losses above the acceptable limits for an economically relevant magnetic fusion power plant. One of the grand challenges of fusion energy science is to understand and control the complex mechanisms responsible for turbulent transport in magnetic confinement devices in order to minimize anomalous transport.

From a theoretical point of view, this is a challenging task. The transport mechanisms are highly nonlinear, and one must find ways computationally to treat the interaction between the vastly separate temporal and spatial scales to properly capture the close coupling between the slow (~ 1 s) evolution of large scale (~ 1 m) variations in density, temperature, and flow profiles, and the rapid (~ 1 MHz) fluctuations of small-scale ($\sim 10^{-5}$ m) plasma turbulence.

A natural way to deal with this difficulty is to exploit the space and time scale separation between mean and fluctuation dynamics by first solving for the microturbulence on a fine space-time mesh, and then using the microturbulent fluxes to self-consistently evolve the mean plasma density, flow, and pressure on a coarser space-time grid. Such an approach has been tested recently, and promising results were obtained [1, 2]. Even if so, the applicability of these numerical solvers to understand and predict experimental results remains limited, for several reasons. First, the multi-scale codes do not yet incorporate all the physical mechanisms occuring at the various spatial and temporal scales in fusion plasmas. Second, there is a partial lack of self-consistency in the sense that the background magnetic field is not allowed to evolve in the simulations, even though the macroscopic profiles change. Third, the computation of the microturbulent fluxes through the numerical solution of nonlinear five-dimensional equations remains expensive computationally.

We spent a large part of the award period developing numerical solvers to address the last two points. In this section, we will present our work on the development of high-performance MHD equilibrium solvers designed to compute the background magnetic configuration consistent with the pressure and velocity profiles obtained from the transport codes at each slow-scale time step. In Section 2, we will discuss numerical methods we designed to accelerate the computation of the turbulent transport fluxes using continuum schemes.

1.1 High performance equilibrium solvers

The need for high performance equilibrium solvers for integrated transport simulations can be understood as follows. First, transport in a tokamak core does not only depend on the magnetic flux function, but also on its derivatives, up to second order. We therefore need a solver able to compute these second derivatives with high accuracy. Second, plasma profiles are not uniform, and regions of strong gradients need to be resolved with more accuracy than regions with flatter profiles. Adaptive refinement is a powerful method in such a case, but unfortunately often leads to numerical ill-conditioning in finite element (FEM) and finite difference (FD) solvers. Third, the equilibrium solvers need to have flexibility in order to accommodate all the different reactor cross-sections that will be studied. They need to work in a robust manner for up-down asymmetric and/or reverse D shaped tokamaks. Finally, the interplay between plasma rotation and turbulent transport in axisymmetric devices is known to have crucial consequences on particle and energy confinement [3] and has triggered much interest in the transport community. There is an ongoing effort to include the physics terms associated with strong flows in the most advanced microturbulence codes, and MHD equilibrium solvers that are to be coupled with these codes have to be able to handle flows in a robust way.

The Grad-Shafranov equation as a nonlinear Poisson problem

The magnetic configuration of static equilibria in axisymmetric devices is determined by solving the Grad-Shafranov equation for the poloidal magnetic flux function ψ:

$$R\frac{\partial}{\partial R}\left(\frac{1}{R}\frac{\partial\psi}{\partial R}\right)+\frac{\partial^2\psi}{\partial Z^2}=-\mu_0 R^2\frac{dp}{d\psi}-\frac{1}{2}\frac{dg^2}{d\psi}\quad \text{in } \Omega\ ,\ \psi=0\quad \text{on } \partial\Omega \tag{1}$$

where R measures the major radius, Z the vertical distance from the midplane, $p(\psi)$ is the plasma pressure profile, and $2\pi g(\psi) = -I_p(\psi)$ is the net poloidal current flowing in the plasma and the toroidal field coils. Ω is the computational domain, and $\partial\Omega$ is the boundary of Ω. In general in magnetic fusion experiments the profile $p(\psi)$ and $g(\psi)$ are such that the right-hand side of the Grad-Shafranov equation is a nonlinear function of the unknown ψ. This means that the Grad-Shafranov equation has to be solved iteratively, independently of the choice of the numerical method. Since iterations are required, we can replace with no additional computational cost the unknown function ψ with another unknown function U defined by $\sqrt{R}U(R,Z)=\psi(R,Z)$. Under this transformation, the Grad-Shafranov equation can be rewritten as

$$\Delta U=-\mu_0 R^{3/2}\frac{dp}{dU}-\frac{1}{2\sqrt{R}}\frac{dg^2}{dU}+\frac{3}{4R^2}U\quad \text{in } \Omega\ ,\ U=0\quad \text{on } \partial\Omega \tag{2}$$

where $\Delta := \partial^2/\partial R^2+\partial^2/\partial Z^2$ is the Cartesian Laplacian operator. In other words, the Grad-Shafranov equation can be seen as a nonlinear Poisson problem, and advanced numerical methods for Poisson's equation can be advantageously applied in plasma physics. This is the basis for the three numerical schemes we describe in the next sections.

Achieving accurate calculations of derivatives with any FEM solver

There has recently been preliminary work investigating the self-consistent coupling between existing FEM based equilibrium solvers and transport codes. Conventional FEM solvers have the disadvantage that once the solution U is computed, derivatives of U are evaluated numerically, and an order of convergence is lost for each derivative that is evaluated in this way. A typical FEM solver for the Grad-Shafranov equation with 4^{th} order convergence for U [4] only has second order convergence for the second derivatives of U. Yet despite this weakness, computational plasma physicists who have spent time coding the challenging interfaces between the transport codes and these FEM codes may not be eager to change the equilibrium solver at the heart of their codes. This is the reason why we developed a new numerical method based on integral equations that allows us, *using the same FEM solver*, to calculate all derivatives of U with the same order of convergence as U. The basic idea is to not calculate the derivatives of U from the output of the FEM solver, but instead to use the FEM solver to solve a new *linear* partial differential equation for the derivatives of U.

More specifically, consider the nonlinear Poisson problem

$$\Delta U = F(U) \quad \text{in } \Omega \ \ , \ U = 0 \quad \text{on } \partial\Omega$$

which is the general form for Eq. (2), and imagine one has an FEM solver for this problem. Straightforward differentiation of this equation leads to elliptic equations for the derivatives of U. For example, for the partial derivative with respect to R, we have

$$\Delta U_R = F'(U)U_R$$

With U known, this equation is linear in U_R, and easy to solve with the same FEM solver as U. One might then think that using the same elements as the ones used to compute U, one can achieve the same order of accuracy for U_R as for U. This is obviously not true in general because one needs a boundary condition for U_R on $\partial\Omega$, which requires taking numerical derivatives. This can lead to significant accuracy loss if one takes derivatives normal to the surface.

However, using an integral equation formulation, we are able to calculate the boundary conditions on the derivatives of U without ever taking derivatives normal to the boundary. The method relies on considering the conjugate gradient V of U and on using Green's second identity to derive an integral equation of the second kind for V on $\partial\Omega$. After solving this integral equation for V with high-order quadrature rules, we can compute spectrally accurate tangential derivatives of V on the boundary. Indeed, since V is periodic along the boundary, simple Fourier methods are fast and spectrally accurate. And since V is the conjugate gradient of U, this is equivalent to computing normal derivatives of U with spectral accuracy, which is precisely what is needed!

We tested our new method for nonlinear Poisson problems on arbitrary smooth domains, which we solved with the same cubic Hermite polynomials as in the popular code CHEASE [4]. We successfully demonstrated that the first and second derivatives could indeed be calculated with the same order of accuracy as the solution itself, as shown in Figure 1.

The details and results of this work are presented in the following article:

L.F. Ricketson, A.J. Cerfon, M. Racch, and J.P. Freidberg, Accurate Derivative Evaluation for any Grad-Shafranov Solver, *Journal of Computational Physics* **305**, 744 (2016)

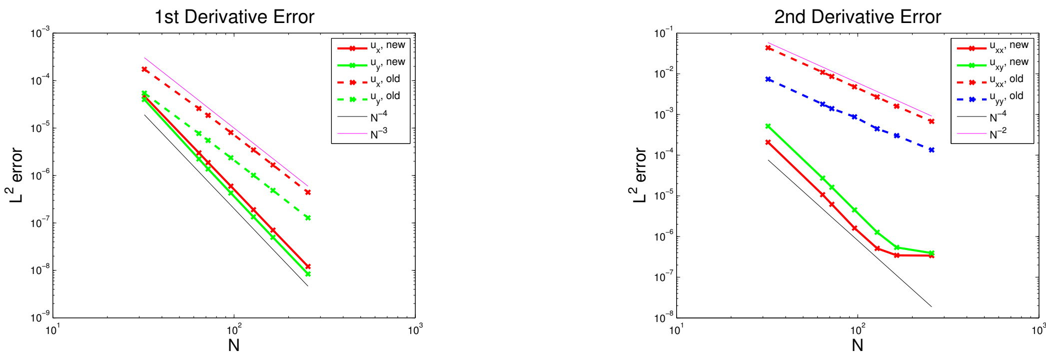


Figure 1: Error in the first and second derivatives of U as a function of the number N of grid points, using two different methods: 1) direct differentiation as usually done in FEM formulations (labeled "old" in the figures), 2) the integral equation formulation we recently developed (labeled "new" in the figures). Observe the significant improvement in the numerical error obtained with our new method.

ECOM: a conformal mapping based fast and spectrally accurate solver for toroidal axisymmetric MHD equilibria

It is our intention to develop in the near future our own code coupling an MHD equilibrium solver with a turbulent transport solver. Since this will not be done starting from an existing framework but instead from scratch, we are free to build our own equilibrium solvers for that purpose, with the idea that they may have improved performance as compared to existing FEM-based solvers, both in terms of speed and accuracy, at least regarding the first and second derivatives of the solution. This is precisely what we did, with the results described below.

The first idea we pursued was to use a spectrally accurate conformal mapping scheme based on the Kerzman-Stein integral equation to map the Poisson equation (2) on the plasma domain Ω to a Poisson equation on the unit disk. We could then solve the Poisson equation on the unit disk by combining a Fourier representation in the polar angle θ with a Green's function solution to the resulting radial ordinary differential equation for each angle θ. By using a piecewise Chebyshev grid for the radial variable and a high-order quadrature rule to evaluate the Green's function convolutions, we achieve spectral convergence for the solutions, as can be seen in Figure 2. Another advantage of combining Fourier and integral equation methods is that derivatives of the solution are not computed by differentiating the solution numerically, and instead evaluated from closed form expressions that can be analytically derived in the integral formulation. As a result, we obtain the same order of convergence for the solution of the Poisson problem as for its derivatives, as can also be seen in Figure 2.

When we compare the performance of our equilibrium solver based on conformal mapping, called ECOM, with the popular finite element solver CHEASE [4], we find that ECOM is much faster than CHEASE for the same number of grid points. This is due to a run-time complexity that is more favorable in ECOM than in CHEASE: unlike CHEASE, ECOM is in the category of fast solvers, with a run time complexity $O(N \log N)$, where N is the number of discretization points. However, because of the crowding effect that is inherent to the conformal mapping technique, the angular grid resulting from the inverse map of the equispaced θ grid on the unit disk typically underresolves certain regions of Ω and requires us to use more grid points than CHEASE to achieve a certain level of accuracy. Despite this limitation, we find that for fusion relevant domains Ω and medium to large grids, ECOM is significantly more accurate than CHEASE for a given run time [5].

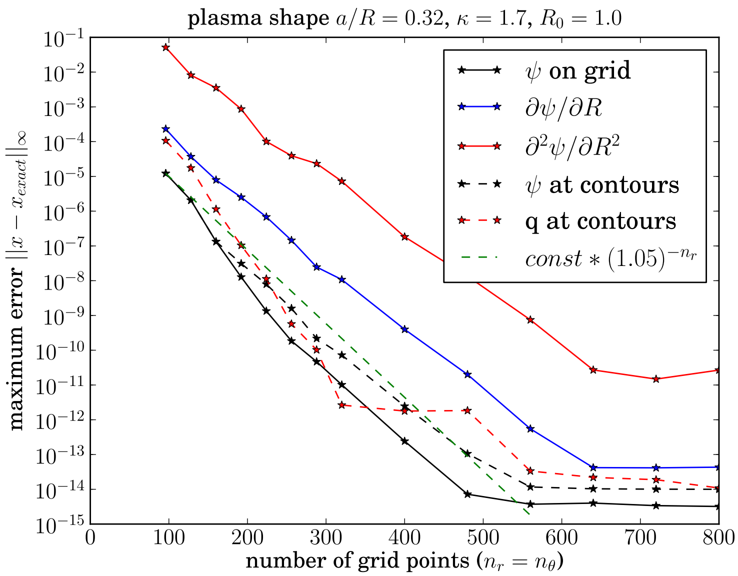


Figure 2: Maximum error between the numerical solution and the known solution for a Solov'ev MHD equilibrium [6]. Observe the geometric convergence for all the physical quantities.

For quantities that depend on the second derivatives of the solution to the equilibrium equation, this is even true for any grid size.

The interplay between plasma rotation and turbulent transport in axisymmetric devices is known to have important consequences on particle and energy confinement [3]. When the macroscopic flows in the plasma are purely in the toroidal direction, the MHD equilibrium is described by a close variant of Eq.(1). We have included an option in ECOM that allows it to compute numerical equilibria with arbitrary toroidal flow.

The details of this work are described in two published articles:

- A.Pataki, A.J. Cerfon, J.P. Freidberg, L.Greengard, M. O'Neil, A fast, high-order solver for the Grad-Shafranov equation, *Journal of Computational Physics* **243**, 28 (2013) – *Supported by other DOE award*
- J.P. Lee and A.J. Cerfon, ECOM: a fast and accurate solver for toroidal axisymmetric MHD equilibria, *Computer Physics Communications* **190**, 72 (2015) – *Supported by other DOE award*

ECOM has recently been used as the equilibrium solver for MHD stability and transport studies in tokamaks. Specifically, it was used to determine the maximum elongation of the plasma cross section that could be stably controlled by feedback systems, following a theoretical framework we developed with J.P. Freidberg (MIT) under this award. Thanks to the speed of ECOM and of our framework, we were able to conduct multiple scans leading to analytic scaling relations for the maximum elongation as a function of the key dimensionless parameters in the problem. These stability studies are presented in:

- J.P. Freidberg, A.J. Cerfon, and J.P. Lee, Tokamak elongation: how much is too much? Part 1. Theory, *Journal of Plasma Physics* **81**, 515810607 (2015)

- J.P. Lee, A.J. Cerfon, J.P. Freidberg, and M. Greenwald , Tokamak elongation: how much is too much? Part 2. Numerical Results, *Journal of Plasma Physics* **81**, 515810608 (2015)
- J.P. Lee, J.P. Freidberg, A.J. Cerfon, and M. Greenwald, An analytic scaling relation for the maximum tokamak elongation against n=0 MHD resistive wall modes, *Nuclear Fusion* **57**, 066051 (2017)

ECOM was also used by turbulence specialists to determine how the shape of the plasma boundary influences the equilibrium magnetic configuration, which in turn influences the nature of the plasma turbulence, and the corresponding transport of momentum. Details of this work, also partially supported by this award, can be found in:

J. Ball, F.I. Parra, J.P. Lee, and A.J. Cerfon, Effect of the Shafranov shift and the gradient of β on intrinsic momentum transport in up-down asymmetric tokamaks, *Plasma Physics and Controlled Fusion* **58**, 125015 (2016)

As mentioned previously, we are now working toward integrating ECOM within a whole device, multi-scale modeling framework for use in optimization and transport studies.

An adaptive fast multipole accelerated Poisson solver for complex geometries

While satisfactory in a wide range of situations, ECOM has weaknesses. Its main disadvantage is that the mesh is not adaptive in the angle variable θ and that the crowding effect for the angular discretization due to the conformal mapping limits the accuracy and speed of the solver as the region Ω becomes too distorted or elongated. While this problem is not significant when simulating existing high aspect ratio tokamak experiments or ITER, it leads to suboptimal performance for low aspect ratio devices or theoretical studies of innovative devices with unusually distorded domains Ω that may have improved transport and/or stability properties [7]. More importantly, the conformal mapping technique is ill-suited numerically for domains that have a corner, a situation that is quite common in magnetic confinement fusion devices and which corresponds to a separatrix of the magnetic field, also known as a magnetic X-point.

To address these challenges, we developed another solver, based on a different integral equation formulation. Consider a given source function f on the domain Ω and the generic Poisson problem

$$\Delta U = f \qquad \text{in } \Omega \ , \qquad U = 0 \ \text{ on } \partial\Omega \tag{3}$$

We solve Eq.(3) as follows. We decompose the solution into a particular solution U^p that solves the differential equation but not for the desired boundary condition, and a homogeneous solution U^h that solves Laplace's equation for the corrected boundary conditions:

$$U = U^p + U^h$$

where U^p is given by

$$U^p(\mathbf{x}) = \frac{1}{2\pi}\int_\Omega f(\mathbf{y})\ln(|\mathbf{x}-\mathbf{y}|)d\mathbf{y} \tag{4}$$

and U^h solves

$$\Delta U^h = 0 \qquad \text{in } \Omega \tag{5}$$

$$U^h = -U^p\big|_{\partial\Omega} \qquad \text{on } \partial\Omega \tag{6}$$

In our solver, we express U^h in terms of the following integral formulation:

$$U^h = \frac{1}{2\pi}\int_{\partial\Omega} \mu(\mathbf{y})\ln(|\mathbf{x}-\mathbf{y}|)d\mathbf{y} + \frac{1}{2\pi}\int_{\partial\Omega} \mu(\mathbf{y})\frac{\partial}{\partial_{\nu_{\mathbf{y}}}}\ln(|\mathbf{x}-\mathbf{y}|)d\mathbf{y} \tag{7}$$

$$\frac{1}{2}\mu(\mathbf{x}_0) - \frac{1}{2\pi}\int_{\partial\Omega} \mu(\mathbf{y})\ln(|\mathbf{x}_0-\mathbf{y}|)d\mathbf{y} - \frac{1}{2\pi}\int_{\partial\Omega} \mu(\mathbf{y})\frac{\partial}{\partial_{\nu_{\mathbf{y}}}}\ln(|\mathbf{x}_0-\mathbf{y}|)d\mathbf{y} = -U^p(\mathbf{x}_0) \tag{8}$$

where $\partial_{\nu_{\mathbf{y}}}$ represents the partial derivative in the direction normal to the boundary. Once again, the advantage of a formulation based on Eqs. (4), (7), and(8) is that derivatives can be expressed explicitly by differentiating under the integral signs.

There exists several high performance codes to compute μ in (8). We used generalized Gaussian quadrature [8, 9] to approximate the integrals and a fast direct solver [10] to compute the density μ. U^h is then computed from Eq.(7), relying on the Quadrature By Explansion (QBX) scheme [12] to obtain high accuracy for the singular integrals, which we accelerated with the Fast Multipole Method [11].

The main challenge in our formulation is to find an efficient method to evaluate the particular solution in (4) accurately and in optimal time. The Fast Multipole Method is known to be specifically designed to calculate convolutions of the type given in Eq. (4) accurately and in optimal time, but the most efficient 2D FMM codes require the knowledge of f on a scaled unit square, and we are only given f in the plasma domain Ω. One therefore needs a strategy to extend f beyond Ω to the boundaries of the unit square domain Ω_B. A naive extension consists in setting $f = 0$ in $\Omega_B \setminus \Omega$. Such an approach is however not satisfying, for two reasons: 1) it limits the order of convergence of the solver if $f \neq 0$ on $\partial\Omega$; 2) high accuracy can only be reached by adaptively discretizing the neighborhood of the boundary $\partial\Omega$ with a large number of leaf boxes, which is computationally costly and inefficient (See figure 4).

We proposed a new strategy to tackle this problem: we construct a global C^0 extension f_e of f outside of the domain Ω by solving the following harmonic problem in the exterior of Ω:

$$\Delta w = 0 \qquad \text{in } \mathbb{R}^2 \setminus \Omega \tag{9}$$

$$w = f \qquad \text{on } \partial\Omega \tag{10}$$

The function f_e defined by

$$f_e(\mathbf{x}) = f(\mathbf{x}) \text{ for } \mathbf{x} \in \Omega$$
$$f_e(\mathbf{x}) = w(\mathbf{x}) \text{ for } \mathbf{x} \in \Omega_B \setminus \Omega$$

is globally continuous, as smooth as f on Ω, and smooth on $\Omega_B \setminus \Omega$. We thus use f_e in place of f in Eq.(4). While this may at first seem like a computationally expensive way to extrapolate f, the analytical and numerical tools required to solve this problem are in fact the same as those required to solve the harmonic problem (7)–(8), which we described above, and therefore have the same run-time complexity [11].

The numerical scheme we propose here for the Poisson problem (3) may be classified as an *embedded boundary method*. This approach is desirable for a “black box” Poisson solver, i.e. a Poisson solver designed to be flexible and robust when used by external users in a variety of applications (such as plasma physics, our main motivation): it guarantees domain flexibility and ease of use, in the sense that all the user has to provide to obtain an accurate answer is a parametric description of the boundary and a method for evaluating f accurately in the domain. As always with an embedded boundary approach, the ease of use has a cost in terms of convergence order. However, adaptive refinement improves the accuracy we achieve per degree of freedom, particularly

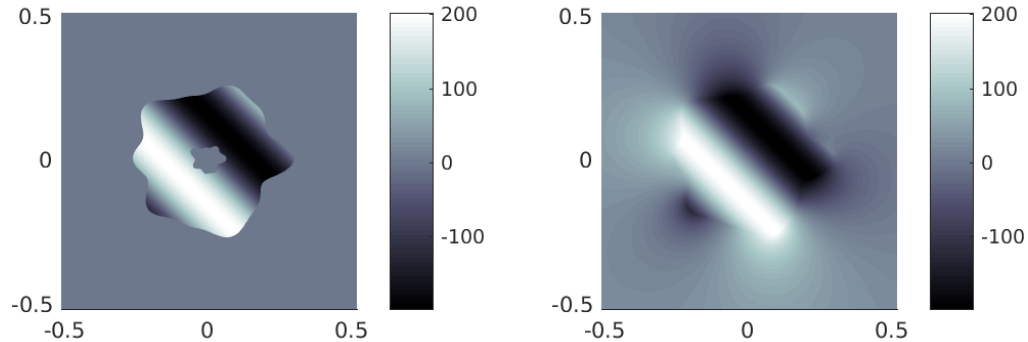


Figure 3: Extended density f_e using extension by zero (left) and continuous extension (right)

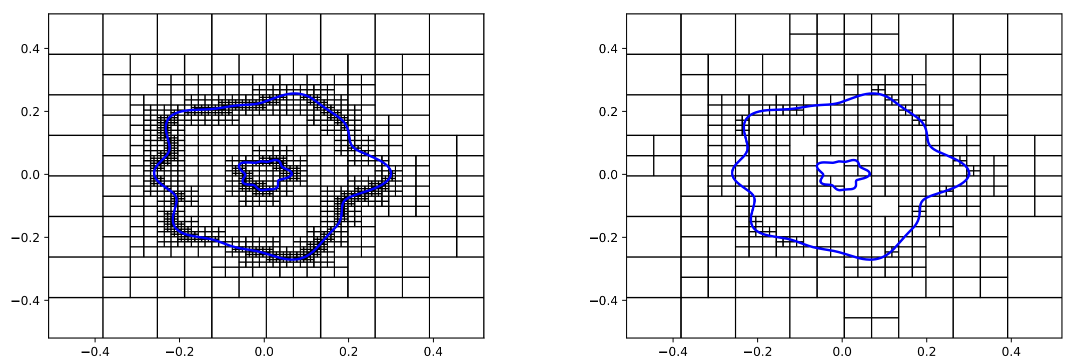


Figure 4: Quad trees used for the FMM accelerated evaluation of the volume potential U^p for the source function f_e shown in Figure 3. The computational domain Ω is the region between the two blue curves. For the example on the left, we extended f by 0 outside of Ω, while for the example on the right, we extended f using our new scheme for continuous extension. Observe the dramatically smaller number of boxes required to discretize the edge of Ω, leading to a much faster and efficient evaluation of U^p for a desired accuracy.

for the gradient. And since we rely on the FMM for the evaluation of (4), the amount of work still scales linearly with the number of degrees of freedom in the computational domain and is competitive with classical FFT-based solvers in terms of work per grid point, despite the flexibility of adaptive mesh refinement. The numerical tests we ran for irregular domains Ω which are multiply connected (see Figures 3 and 4) numerically confirmed the flexibility, accuracy, and efficiency of our scheme [11].

The details of this work can be found in the following published article:

T. Askham and A.J. Cerfon, An adaptive fast multipole accelerated Poisson solver for complex geometries, *Journal of Computational Physics* **344**, 1 (2017)

Adaptive Hybridizable Discontinuous Galerkin discretization of the Grad-Shafranov equation

There are strong mathematical reasons suggesting that integral equation formulations indeed lead to the most robust and efficient codes for magnetic equilibrium calculations in fusion devices.

However, this field of numerical mathematics is not as mature as other fields, and certain situations can therefore not yet be easily treated with integral equations. This is in particular the case when the plasma boundary has an X-point, corresponding to a divertor.

In order to have an efficient and robust solver for these cases, and waiting for readily available approaches with integral equations, we proposed a scheme based on the hybridizable discontinuous Galerkin (HDG) method. Our approach has the originality of sidestepping the usual need for geometry-conforming triangulations, thanks to a transfer technique that allows to approximate the solution using only a polygonal subset as computational domain. Moreover, the solver features automatic mesh refinement driven by a residual-based a posteriori error estimator. As the mesh is locally refined, the computational domain is automatically updated in order to always maintain the distance between the actual boundary and the computational boundary of the order of the local mesh diameter. We demonstrated extensive numerical evidence of the suitability and efficiency of our method for physically relevant equilibria with pressure pedestals, internal transport barriers, and current holes on realistic geometries. An example with a current hole is shown in Figure 5, where the adaptive refinement in the vicinity of the plasma edge is clearly visible.

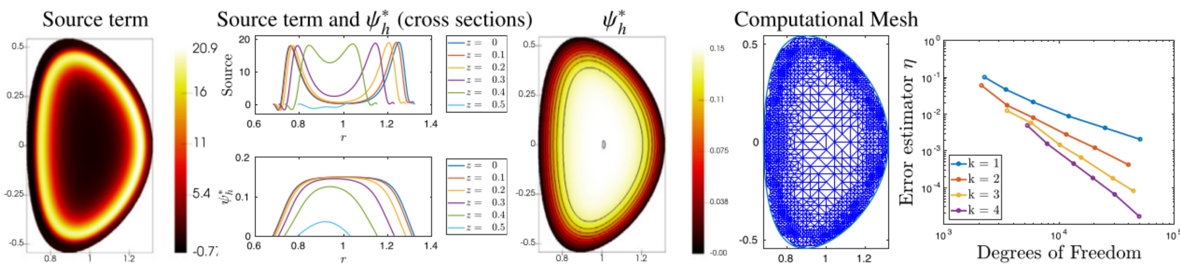


Figure 5: Source term for an equilibrium with a current hole (first and top-second panels). This gives rise to mesa-like magnetic flux function (second- bottom and third panels). The refinement is automatically driven towards the boundary (fourth panel). The solution is updown symmetric and only cross sections for the upper half are plotted.

The details of this work can be found in:

T. Sanchez-Vizuet, M.E. Solano, and A.J. Cerfon, Adaptive Hybridizable Discontinuous Galerkin discretization of the Grad-Shafranov equation by extension from polygonal subdomains, *Computer Physics Communications* **255**, 107239 (2020)

1.2 Fast integral equation based Beltrami solvers for the computation of three-dimensional MHD equilibria

The differential equations for the trajectory of magnetic field lines in any toroidal geometry can be written in the form of canonical equations for a one-and-a-half-degree-of-freedom Hamiltonian, where the toroidal angle ζ plays the role of time [14]. In devices with toroidal axisymmetry, any equilibrium quantity is independent of ζ, and so is the Hamiltonian. This makes the Hamiltonian system integrable, and guarantees the existence, throughout the plasma, of nested toroidal surfaces corresponding to contours of constant magnetic flux. These contours are given by the Grad-Shafranov equation (1), which was the focus of section 1.1. In contrast, if toroidal axisymmetry is lost, the Poincaré map of magnetic field lines, computed for example by recording the location of magnetic field lines as they cross the plane $\zeta = 0$, may show chaotic regions and resonant island chains along with regular trajectories [14, 15]. This makes the design of robust MHD solvers for general three-dimensional equilibria remarkably difficult, and complicates the analysis of experimental equilibria.

A recent, promising approach to capture many of the intricacies of plasma equilibria in three-dimensional devices is to subdivide the plasma into separate regions assumed to have undergone Taylor relaxation [16] to a minimum energy state subject to conserved fluxes and magnetic helicity, and separated by ideal MHD barriers [17, 18, 19]. The numerical code based on this formulation, called SPEC [20], is able to reproduce several of the key features of three dimensional equilibria, and has given very promising results thus far.

As a result of Taylor relaxation, the magnetic field in SPEC is force-free in each region Ω and satisfies

$$\nabla \times \mathbf{B} = \lambda \mathbf{B} \ \text{ in } \Omega \ , \quad \mathbf{B} \cdot \mathbf{n} = 0 \ \text{ on } \partial\Omega \tag{11}$$

where λ is a constant in each region, and $\mathbf{n}$ is the outward unit normal vector to the boundary $\partial\Omega$. For uniqueness of the solution, Eq.(11) has to be supplemented with flux conditions: one flux condition if the genus of Ω is one, two flux conditions if the genus of Ω is two. Fields satisfying Eq.(11) are often called linear Beltrami fields. We have developed a new solver for linear Beltrami fields in toroidal geometries, with the magnetic fluxes given as constraints and λ specified as an input. The solver relies on an integral formulation for the force-free fields that is based on the generalized Debye source representation for electromagnetic fields [21].

In order to understand the link between the generalized Debye source representation and Eq.(11), observe that if a magnetic field $\mathbf{B}$ satisfies (11), then the pair $\{\mathbf{E}, \mathbf{H}\}$ defined by

$$\mathbf{E} := i\mathbf{B} \ \ , \ \ \mathbf{H} := \mathbf{B}$$

satisfies the time-harmonic Maxwell's equations in vacuum, with λ playing the role of the wave number k. Furthermore, the boundary condition $\mathbf{B}\cdot\mathbf{n} = 0$ translates to the two boundary conditions $\mathbf{E} \cdot \mathbf{n} = 0$ and $\mathbf{H} \cdot \mathbf{n} = 0$ on $\partial\Omega$. In other words, we can apply the generalized Debye source representation originally developed for electromagnetic scattering from perfect conductors for the computation of linear Beltrami fields. Specifically, we represent $\mathbf{B}$ as

$$\mathbf{B} = i\lambda\mathbf{Q} - \nabla v + i\nabla \times \mathbf{Q} \tag{12}$$

where $\mathbf{Q}$ and v are generalized Debye potentials [21], which themselves can be expressed as layer potentials $\mathbf{m}$ and σ along $\partial\Omega$:

$$\mathbf{Q}(\mathbf{x}) = \int_{\partial\Omega} \frac{e^{i\lambda|\mathbf{x}-\mathbf{x}'|}}{4\pi|\mathbf{x}-\mathbf{x}'|}\mathbf{m}(\mathbf{x}')dA' \qquad v(\mathbf{x}) = \int_{\partial\Omega} \frac{e^{i\lambda|\mathbf{x}-\mathbf{x}'|}}{4\pi|\mathbf{x}-\mathbf{x}'|}\sigma(\mathbf{x}')dA'$$

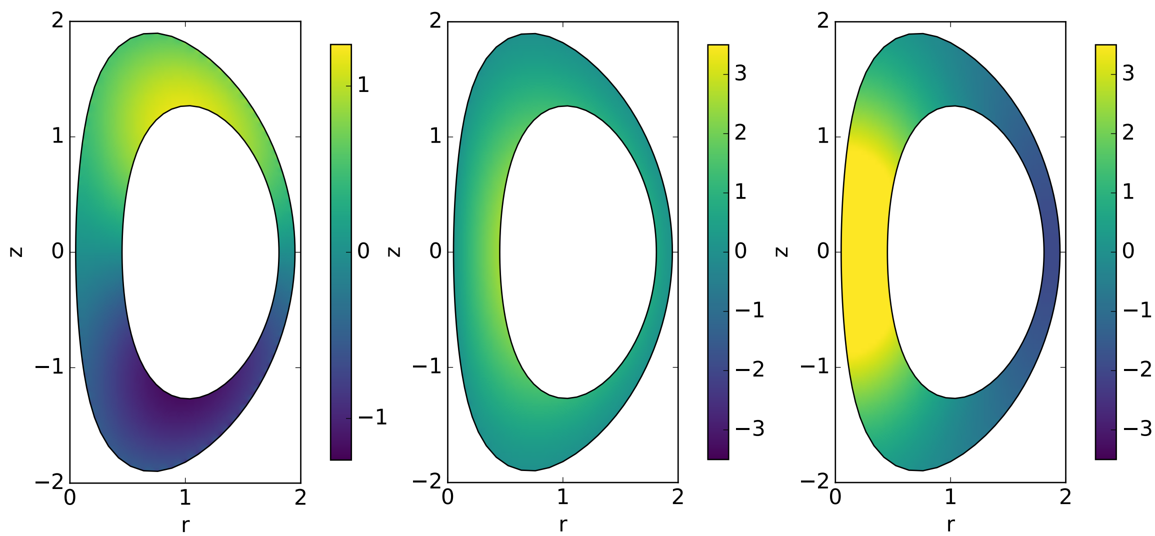
This representation leads to a well-conditioned (away from physical resonances) second-kind integral equation for σ which can be numerically inverted to high-precision [22]. Once σ is known, $\mathbf{m}$, and thus $\mathbf{Q}$ and v can be computed by direct numerical evaluation.

This formulation has the following advantages:

- The solver has low memory requirements, since the unknowns in the integral equation are defined on the boundary of the domain only
- Since the interior of the domain does not need to be discretized, high accuracy is reached with a modest number of unknowns, even with highly distorted or low aspect ratio, highly elongated domains (see domain considered in Figure 6)

- In the context of SPEC, in which the locations of the ideal interfaces of each force-free region are iteratively updated until force balance is satisfied at each boundary, our formulation gives the possibility to apply the entire iterative procedure by discretizing the ideal interfaces only, and the converged global magnetic field would only be evaluated in the entire domain at the very end, once global force balance has been reached

We have tested our solver for toroidally axisymmetric boundaries $\partial\Omega$, comparing the numerical results with exact equilibria computed for complex geometries (see Figure 6) [23]. We numerically demonstrated that one obtains high accuracy with a modest number of unknowns and small run time.



(a) B_r (b) B_θ (c) B_z

Figure 6: Components of the Beltrami field $\mathbf{B}$ in cylindrical coordinates, for a toroidal shell with very low aspect ratio.

The following two articles discuss this work in more detail:

- A.J. Cerfon and M. O'Neil, Exact axisymmetric Taylor states for shaped plasmas, *Physics of Plasmas* **21**, 064501 (2014) – *Supported by other DOE award*
- M. O'Neil and A.J. Cerfon, An integral equation-based numerical solver for Taylor states in toroidal geometries, *Journal of Computational Physics* **359**, 263 (2018)

After testing our solver in axisymmetric domains, we extended it in order to solve equilibria with nonaxisymmetric boundaries. This enabled us to incorporate our code in the SPEC framework.

Our results initially showed much improved performance as compared to the SPEC solver, in terms of accuracy and robustness. These results motivated the SPEC developer to further optimize their solver, which now is faster than our solver. We plan to continue the development of our codes in parallel, to provide the community with two competitive solvers, which each have advantages and disadvantages. An example Beltrami magnetic field computed with our approach in a general non-axisymmetric domain can be found in Figure 7. Further details can be found in:

D. Malhotra, A.J. Cerfon, L.-M. Imbert-Gérard, and M. O'Neil, Taylor States in Stellarators: A Fast High-order Boundary Integral Solver, *Journal of Computational Physics* **397**, 108791 (2019)

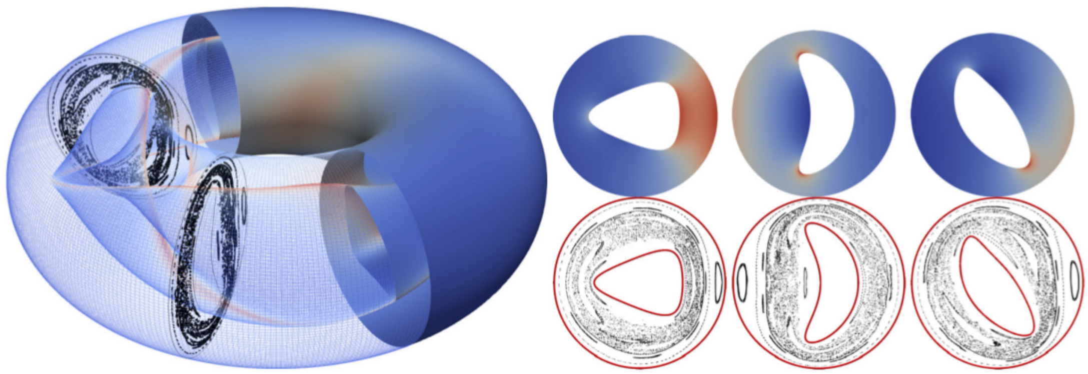


Figure 7: An example of a Taylor state computed in a toroidal-shell domain. Using our boundary integral method, we only need to discretize the domain boundary. This reduces the dimensionality of the of unknowns needed, and leads to significant savings in computational work. Once the boundary integral equations is solved, the magnetic field **B** can be evaluated at off-surface points very efficiently. On the right, we show the magnitude of **B** in different cross-sections of the domain as well as Poincar plots of the field in each cross section, generated by tracing the field lines.

By-product: Efficient high-order singular quadrature schemes in magnetic fusion

Our integral formulation for the computation of Beltrami fields requires the numerical evaluation of integrals with singular kernels. It turns out that such integrals occur in several other fusion applications, such as the Virtual Casing Principle [24, 25]. The quadrature scheme we implemented in our Beltrami solver for these integrals is significantly more accurate than quadrature schemes proposed by the fusion community for these other applications, which we demonstrated in the following article:

D. Malhotra, A.J. Cerfon, M. O'Neil, and E. Toler, Efficient high-order singular quadrature schemes in magnetic fusion, *Plasma Physics and Controlled Fusion* **62**, 024004 (2020) (Special Issue on 3D MHD Equilibria: Flux Surfaces, Islands and Chaotic Fields)

Our quadrature scheme is currently implemented for all these applications in the new stellarator optimization code Simsopt.

2 Discretization scheme for the speed variable in kinetic solvers

Solving the kinetic equations describing plasma microturbulence numerically is computationally intensive, so an important aspect of the theoretical effort in this field is to find new optimized discretization schemes. While high order accurate discretization schemes for the spatial variables have been successfully used for many years, finding an ideal discretization method remains challenging for the discretization of velocity space in situations involving Fokker-Planck collisions [26]. Since the Fokker-Planck collision operator has terms involving first and second order derivatives with respect to the velocity variables, the discretization method must allow accurate differentiation. The scheme must also allow accurate integration since physical quantities such as the number density, the mean fluid velocity and the pressure depend on velocity moments of the distribution function.

Recently, promising new approaches based on spectral and pseudo-spectral representations have been investigated [27] and [28]. It was shown in [27] that a Hermite representation for the parallel velocity has advantages over the more common finite difference schemes used in numerical simulations. In [28], different representations for the speed coordinate are explored for some important steady-state equations in plasma physics. It is found that because the variable has values in $[0, \infty)$ instead of the entire real axis, a little-known family of non-classical polynomials called *Maxwell polynomials* [29, 30, 31] which are orthogonal with respect to the weight function $x^2 e^{-x^2}$ on the half-line gives much better performance than finite difference schemes and schemes based on classical orthogonal polynomials. High accuracy is obtained on very coarse grids for both differentiation and integration of Maxwell-Boltzmann like functions, which are the functions of interest in many applications of interest in plasma physics [28].

We decided to look at the suitability of Maxwell polynomials for initial-value calculations of turbulent transport in the presence of collisions. To do so, we considered a model one-dimensional problem describing energy diffusion due to FokkerPlanck collisions given by

$$\frac{\partial f}{\partial t} = \frac{1}{v^2}\frac{\partial}{\partial v}\left[\Psi(v) v^2 e^{-v^2}\frac{\partial}{\partial v}\left(e^{v^2} f\right)\right] , \qquad v > 0, t > 0 \tag{13}$$

with

$$\Psi(v) = \frac{1}{2v^3}\left[\mathrm{erf}(v) - \frac{2}{\sqrt{\pi}} v e^{-v^2}\right] \ , \ \mathrm{erf}(v) = \frac{2}{\sqrt{\pi}}\int_0^v e^{-u^2} du$$

We chose this model problem because the right-hand side of Eq.(13) is the speed variable piece of the energy diffusion operator in the Landau-Fokker-Planck operator for same-species collisions [32]. It it therefore directly relevant to plasma microturbulence simulations.

Our work on Eq.(13) was split in two parts. First, we constructed an exact solution to Eq.(13) in order to be able to assess the *absolute* accuracy of the numerical discretization schemes we will propose to solve that equation. Analytic solutions to Eq.(13) for physically relevant initial conditions are not known. We thus developed a highly accurate but expensive method to compute solutions to this equation and serve as a reference point for less accurate but faster numerical schemes. The method is based on representing the solution as a discrete and continuous superposition of normalizable and nonnormalizable eigenfunctions via the spectral transform of the singular Sturm–Liouville operator associated with Eq.(13). The spectral density function of the operator is computed with a new algorithm that uses Chebyshev polynomials to extrapolate the value of the Titchmarsh–Weyl m-function from the complex upper half-plane to the real axis.

More details of this work can be found in:

J. Wilkening and A.J. Cerfon, A Spectral Transform Method for Singular Sturm–Liouville Problems with Applications to Energy Diffusion in Plasma Physics, *SIAM Journal of Applied Mathematics* **75**, 350 (2015) – *Supported by other DOE award*

In the second step, we solved Eq.(13) through direct numerical discretization of the equation. We considered two approaches. The first approach aimed at better understanding the approximation properties of Maxwell polynomials for time-dependent problems, and relied on a Galerkin spectral representation for the variable v. We integrated the resulting ordinary differential equations exactly in time in order to focus on spatial discretization. We demonstrated that much higher accuracy is obtained with Maxwell polynomials than with Hermite polynomials or the finite difference scheme currently used in the popular plasma microturbulence code GS2 [33] and AstroGK [34], even for very coarse grids, and provided mathematical explanations for this behavior.

Since spectral approaches and exact time integration can be challenging to implement in the frameworks currently used for the simulation of the nonlinear five-dimensional equations describing

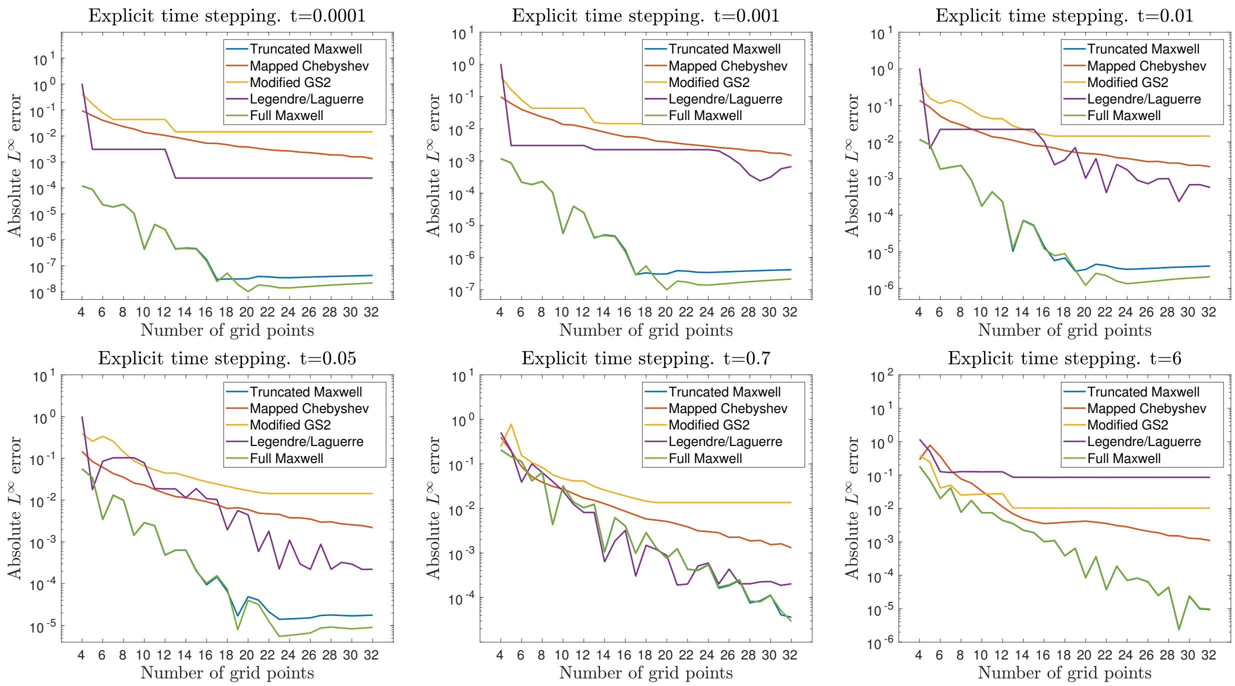


Figure 8: Convergence plots in the L^∞ norm for the solution of Equation (13) with explicit time stepping and initial condition $f_i(x, 0) = x^2 e^{-x^2}$. We observe that Maxwell polynomials lead to much higher accuracy than all other schemes considered, and high accuracy even for small numbers of grid points.

turbulence in plasmas, we also considered a second approach which is usually preferred in these frameworks, namely a velocity discretization scheme based on a pseudo-spectral collocation, and advancing the solution in time with standard time stepping schemes. Doing so, we confirmed that Maxwell polynomials lead to better performance than all other discretization schemes traditionally considered, as shown in Figure 8. We also highlighted two numerical instabilities – an exponential instability and a nonmodal instability – which constrain the form of the pseudospectral differentiation operators which should be used for satisfying performance, and proposed a formulation which is not subject to these instabilities.

This work is summarized in the following articles:

- J. Wilkening, A.J. Cerfon and M. Landreman, Accurate spectral numerical schemes for kinetic equations with energy diffusion, *Journal of Computational Physics* **294**, 58 (2015)
- T. Sanchez-Vizuet and A.J. Cerfon, Pseudo-spectral collocation with Maxwell polynomials for kinetic equations with energy diffusion, *submitted to Plasma Physics and Controlled Fusion*, preprint: arXiv:1708.09031

3 Reduced model for the study of the drift wave - zonal flow paradigm, and of the Dimits shift

The high level of energy transport towards the edge observed in magnetic fusion experiments is responsible for the unsatisfying power balance and insufficient gain factors measured in current fusion devices. As explained in the introduction, it has been found experimentally and confirmed computationally that the strong transport is due to complex turbulent processes driven by plasma microinstabilities. A quantitatively accurate description of turbulence driven transport requires extremely expensive kinetic simulations, with simulation times measured in weeks when they are run on the largest supercomputers. The high computational cost of the kinetic simulations makes it challenging to conduct parametric studies, to quantify uncertainty and sensitivities, and to investigate innovative methods to improve the energy confinement time in magnetically confined plasmas. In that context, reduced fluid models can play a major role, as effective tools to qualitatively understand the fundamental nonlinear processes regulating the turbulence, determine the dependence of energy transport on the key experimental parameters, and identify strategies to reduce the level of transport. In particular Hasegawa-Mima [37] and Hasegawa-Wakatani [38, 39] models have been two very popular simple models to study the interplay between drift wave driven turbulence and zonal flows. Nevertheless, these models remain far from accurately matching the nonlinear processes seen in actual fusion experiments and in expensive simulations based on first principles. We proposed a new reduced fluid model, in the same family as the Hasegawa-Wakatani models [38, 39], which has a better match with experiments, in the sense that it better reproduces the nonlinear upshift away from the linear stability threshold for the onset of significant turbulence driven transport. This upshift is known as the Dimits shift [40], and is thought to play a major role in tokamak transport. Figure 9 shows the difference between the critical linear stability gradient and the onset of significant turbulence driven transport in our balanced Hasegawa-Wakatani (BHW) model.

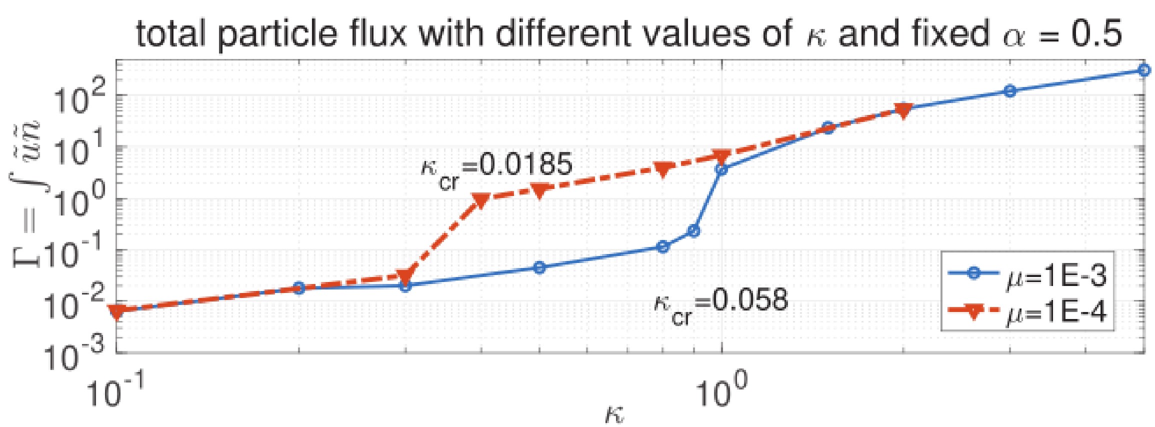


Figure 9: Total radial particle flux Γ in the BHW model as a function of the background density gradient κ for two different values of the collisional diffusion parameter μ. The value of the critical linear stability κ is called $\kappa_{\rm cr}$ and shown for each curve. Our BHW model has a clear nonlinear upshift of the density gradient corresponding to strong turbulence driven transport, similar to the Dimits shift.

Our model is also capable of reproducing several key features of zonal flows observed in more complete models, as well as the existence of solitary propagating structures. A typical time evolution of the zonally averaged mean flow in our model is shown in Figure 10, where we see sparse bursts also observed in more complex models. All these results are presented in the following series of articles:

- D. Qi, A. J. Majda, and A. J. Cerfon, Dimits shift, avalanche-like bursts, and solitary propagating structures in the two-field flux-balanced HasegawaWakatani model for plasma edge turbulence, *Physics of Plasmas* **27**, 102304 (2020) – *Selected as Featured article by Physics of Plasmas*

- D. Qi, A.J. Majda and A.J. Cerfon, A Flux-Balanced Fluid Model for Collisional Plasma Edge Turbulence: Numerical Simulations with Different Aspect Ratios, *Physics of Plasmas* **26**, 082303 108791 (2019)

- A.J. Majda, D. Qi and A.J. Cerfon, A flux-balanced fluid model for collisional plasma edge turbulence: model derivation and basic physical features, *Physics of Plasmas* **25**,102307 (2018)

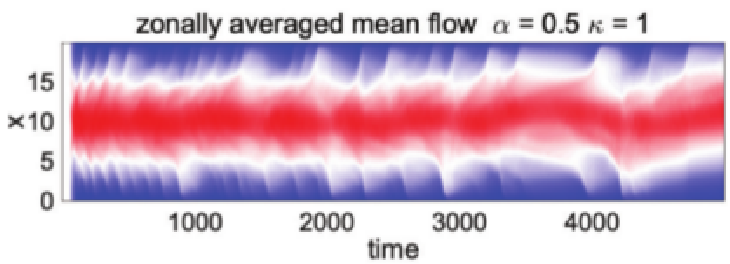


Figure 10: Time evolution of the zonal mean velocity in the BHW model. Relatively infrequent bursts are observed.

4 Elimination of MHD current sheets by modifications to the plasma wall in a fixed boundary model

Models of magnetohydrodynamic (MHD) equilibria that for computational convenience assume the existence of a system of nested magnetic flux surfaces tend to exhibit singular current sheets for non-axisymmetric equilibria. These sheets are located on resonant flux surfaces that are associated with rational values of the rotational transform. We studied the possibility of eliminating these singularities by suitable modifications of the plasma boundary, which we prescribed in a fixed boundary setting. We found that relatively straightforward iterative procedures can be used to eliminate weak current sheets that are generated at resonant flux surfaces by the nonlinear interactions of resonating wall harmonics. These types of procedures may prove useful in the design of fusion devices with configurations that enjoy improved stability and transport properties.

More details can be found in:

E. Kim, G.B. McFadden, and A.J. Cerfon, Elimination of MHD current sheets by modifications to the plasma wall in a fixed boundary model, *Plasma Physics and Controlled Fusion* **62**, 044002 (2020) (Special Issue on 3D MHD Equilibria: Flux Surfaces, Islands and Chaotic Fields)

5 Reactor studies to compare pulsed and steady-state tokamaks

We have carried out a detailed analysis that compares steady state versus pulsed tokamak reactors. The motivations are as follows. Steady state current drive has turned out to be more difficult than expected it takes too many watts to drive an ampere, which has a negative effect on power balance and economics. This is partially compensated by the recent development of high temperature REBCO superconductors, which offers the promise of more compact, lower cost tokamak reactors, both steady state and pulsed. Of renewed interest is the reduction in size of pulsed reactors because of the possibility of higher field Ohmic transformers for a given required pulse length. Our main conclusion is that pulsed reactors may indeed be competitive with steady state reactors and this issue should be re-examined with more detailed engineering level studies.

The details of this work can be found in:

D.J. Segal, A.J. Cerfon, and J.P. Freidberg, Steady state versus pulsed tokamak reactors, *Nuclear Fusion* **61** 045001 (2021)

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