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COMPUTATIONAL METHODS FOR STELLERATOR CONFIGURATIONS

FINAL REPORT

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Final Technical Report for Grant DE-FG02-89ER53285

" Computational Methods for Stellarator Configurations"

This project had two main objectives. The first one was to continue to develop computational methods for the study of three dimensional magnetic confinement configurations. The second one was to collaborate and interact with researchers in the field who can use these techniques to study and design fusion experiments.

The first objective has been achieved with the development of the spectral code BETAS and the formulation of a new variational approach for the study of magnetic island formation in a self consistent fashion. The code can compute the correct island width corresponding to the saturated island, a result shown by comparing the computed island width with the results of unstable tearing modes in Tokamaks and with experimental results in the IMS Stellarator (see attached document and figures).

In addition to studying three dimensional nonlinear effects in Tokamaks configurations, these self consistent computed island equilibria will be used to study transport effects due to magnetic island formation and to nonlinearly bifurcated equilibria.

The second objective was achieved through direct collaboration with Steve Hirshman at Oak Ridge, D. Anderson and R. Talmadge at Wisconsin as well as through participation in the Sherwood and APS meetings.

I include a detailed description of the technical aspects as well as computational results in the attached document.

Professor Octavio Betancourt
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I.- Magnetohydrodynamics in fully three dimensional space

The search for solutions of the magnetostatics equations,

$$J \times B = \nabla p, \quad \nabla \times B = J, \quad \nabla \cdot B = 0,$$

where B , p and J stand for the magnetic field, pressure and current density respectively, represents a significant challenge in a fully three dimensional domain. The existence of classical solutions is brought into question by the analysis of KAM theory [1].

We strongly believe that a better approach to this problem is to start from the more basic formulation of a variational principle, rather than from the partial differential equations themselves.

This point of view has been tried and it has been proven successful in a series of numerical computations by Bauer, Betancourt and Garabedian, starting with the sharp boundary model [2] and then extended to the diffuse plasma case [3]. Further development, including application to magnetic confinement devices appeared in [4], with linear and nonlinear stability analysis included in [5] and local mode analysis and stellarator applications in [6]. The transport problem, using numerically computed solutions of the 3D MHD equations was studied in [7, 8, 9].

A significant improvement in numerical accuracy for the equilibrium problem was obtained by Hirshman using spectral techniques [10]. A fast iterative method was developed by Betancourt, which coupled to a spectral representation and a special choice of collocation points in the radial direction, results in greatly enhanced resolution at a greatly reduced computer cost [11,12]. This greater efficiency and accuracy will allow us for the first time to study the more subtle mathematical questions related to non- existence of solutions, destruction of flux surfaces, island formation and ergodic regions.

This new code was applied to the computation of bifurcated equilibrium solutions in Tokamaks and Stellarators [13], and the new numerical techniques were incorporated to the Oak Ridge spectral code [14]. Work currently in progress deals with a variational formulation to study bifurcation with respect to changes in the topology of the flux surfaces, with future work planned on the effect of island formation on confinement properties in magnetic confinement devices [15].

II.- Magnetic Field Representation

Our formulation of the variational principle of magnetohydrodynamics is based upon a representation of the magnetic field B , defined in a toroidal region Ω and satisfying $\nabla \cdot B = 0$ in terms of a sum of Clebsch potentials [16] of the form,

$$B = \nabla\theta \times \nabla s + \nabla\psi \times \nabla v, \quad (1)$$

where s and ψ are single valued potentials representing the toroidal and poloidal fluxes respectively. We assume that the surfaces $s=\text{constant}$ are a nested family of tori, with $s=1$ corresponding to the boundary of the domain Ω and $s=0$ to a curve in space known as the magnetic axis. The potentials θ and v are angle like variables in the poloidal and toroidal direction, with s the radial coordinate. We can choose one of them arbitrarily and we set $v=\phi$, the toroidal angle. The poloidal flux function ψ is in the most general case a function $\psi(s, \theta, v)$ and it alone determines the basic topological structure of the magnetic surfaces.

It is important to observe that given a divergence free magnetic field B and a fixed choice for v , there is still a degree of freedom in the determination of the potentials s , θ and ψ . They satisfy Hamilton's equations,

$$\frac{ds}{dv} = -\frac{\partial\psi}{\partial\theta}, \quad \frac{d\theta}{dv} = \frac{\partial\psi}{\partial s},$$

and canonical transformations of the Hamiltonian ψ leave the magnetic field invariant. This nonuniqueness of the representation can be a problem for any numerical computation unless it is dealt with properly.

We can distinguish three important cases depending on the functional structure of the poloidal flux function. The simplest is when $\psi = \psi(s)$ is a function of s alone, so that both s and ψ are single valued solutions of the equation,

$$B \cdot \nabla s = 0, \quad B \cdot \nabla \psi = 0,$$

and therefore the set of nested surfaces $s=\text{constant}$ are flux surfaces. This is the key assumption in the formulation of the variational principle and the resulting numerical techniques. This allows us to integrate the equation $B \cdot \nabla p = 0$ by setting $p=p(\psi)$ and thus removing the real characteristics from the magnetostatics equations.

Note that this assumption contradicts the results of KAM theory and Grad's nonexistence conjecture. It is therefore very important to try to gain a deeper analytical understanding of what this means with regards to solutions computed by the variational principle, what mathematical properties do they have and how do they relate to solutions of the partial differential equations. This issues have been considered for the variational principle in one dimension in [17] and for the two dimensional case in [18]. The mathematical properties of the solutions to the variational principle in three dimensions will be one of the main objectives of this proposal, based on the collaboration and interaction between the analytic expertise of Prof. Berger and the numerical and computational experience of Prof. Betancourt.

We can still keep the basic premise of the previous case if we assume that $\psi = \psi(s, \theta)$ is a single valued function of s and θ . It follows that ψ is a flux function satisfying $B \cdot \nabla \psi = 0$ and $p = p(\psi)$ also satisfies $B \cdot \nabla p = 0$.

In this case we assume the existence of a nested set of surfaces $s = \text{constant}$, not necessarily flux surfaces. We introduce poloidal and toroidal angles u and v with periods equal to one and to L on each s surface, and we set

$$\theta(s, u, v) = u - \frac{nv}{mL} + \theta_p, \quad (2)$$

where n, m are integers and θ_p is single valued. Since $m\theta$ has unit periods, we can consider periodic functions of the form

$$\psi(s, \theta) = \sum_k \psi_k(s) e^{2\pi i k m \theta}. \quad (3)$$

The derivative of the poloidal flux to the toroidal flux inside $s = s_0$ is given by

$$\frac{dF}{ds} = \frac{n}{m} + \psi_0'(s_0) = \langle \iota \rangle \quad (4)$$

and measures the average rotational transform $\langle \iota \rangle$ on $s = s_0$. Resonant surfaces are defined by the condition $\langle \iota \rangle = \frac{n}{m}$. We can represent a magnetic island by choosing $\psi_0'(s_0) = 0$ at the resonance, with $\psi_1(s_0) \neq 0$.

The general case, when $\psi = \psi(s, \theta, v)$ is a function of all three variables corresponds to ergodic magnetic lines. That is to say, there are no flux surfaces and a single line covers a volume in space. In this case there is no obvious way to explicitly integrate the equation $B \cdot \nabla p = 0$, except to prescribe $p = \text{constant}$ in the ergodic region. This case is of great importance for Tokamaks, the main design for magnetic confinement devices. Here the nonlinear interaction between two magnetic islands is believed to result in the phenomena known as disruption, where the main plasma volume becomes an ergodic region and the plasma is quickly lost. The problem of interaction of magnetic islands will be another of our research objectives, both the formulation via the variational principle as well as the numerical computation of specific cases relevant to fusion devices.

III.- The Variational Principle

In ideal magnetohydrodynamics, the equilibrium and stability of a plasma with pressure p , confined by a magnetic field B , can be analyzed using a variational principle for the potential energy,

$$E = \int \left(\frac{1}{2} B^2 - p \right) dV,$$

subject to the following constraints :

i.- $\nabla \cdot B = 0$, which we integrate using the magnetic field representation discussed above.

ii.- Fluxes are prescribed, the poloidal flux function $\psi(s, \theta)$ is a given function of s and θ .

iii.- The pressure $p(\psi)$ is a given function of ψ alone. If the flux surfaces are restricted to be nested and $\psi = \psi(s)$, we can prescribe the mass in order to explore compressibility effects on stability.

iv.- The outer wall $s = 1$ is a flux surface, so that the normal component of B vanishes there. This implies $\psi(1, \theta) = \text{constant}$. The more general case where the plasma is bounded by a free surface and surrounded by a vacuum region has also been studied, but will not be described here.

We now look for equilibrium solutions as stationary points of the potential energy, while local minima correspond to stable equilibria. It is possible to compute unstable

equilibria with a descent method by restricting the class of functions admissible in the variation.

For example, we can compute axially symmetric equilibria by assuming the magnetic field to be independent of the toroidal angle v , and then analyze its stability properties by allowing non-axially symmetric perturbations. If found to be unstable, it is possible to find a second solution which is stable to 3D perturbations and globally stable. This is the case of nonlinear bifurcation solutions.

A second example is that of a three dimensional solution which is restricted to have nested flux surfaces, by prescribing the poloidal flux function to be a function $\psi = \psi(s)$. We can then relax this constraint, and examine the stability of the solutions with respect to perturbations of the poloidal flux function by allowing it to depend on θ . If the nested solution is unstable, we will find a second nonlinearly bifurcated solution which will exhibit island formation.

For the computational implementation of the variational principle, it is crucial to choose θ as a dependent variable and s as an independent variable. The latter allows us to express the constraints explicitly and to work on a simple domain in s , v and u coordinates. The former is important to deal with the nonuniqueness of the magnetic field representation, which in the case of nested flux surfaces reduces to an additive function of s in the potential θ . This is not a problem since the expression for B involves only tangential derivatives θ_u and θ_v .

In the more general case when $\psi = \psi(s, \theta)$, the nonuniqueness is not trivial and should be expected to create problems for the numerical algorithm. In practice we consider cases where ψ_θ is small and we are able to compute solutions even when they are not unique. A more satisfactory answer would be to find the appropriate gauge which renders the solution unique. This is still an open problem and another of our research objectives.

IV.- Energy minimization

Having already integrated the two equations $\nabla \cdot B = 0$ and $B \cdot \nabla p = 0$, only two scalar equations are required to satisfy the equilibrium equations. We consider a modified cylindrical coordinate system $A + r, \phi, z$ with A the major radius of the torus and ϕ the toroidal angle. We look for a mapping from s, v, u space onto r, ϕ, z . We are free to

choose v to satisfy $v = A\phi$, with $0 \leq v \leq L = 2\pi A$, $0 \leq u \leq 1$, $0 \leq s \leq 1$. We let $s = 0$ correspond to the magnetic axis and $s = 1$ to the outer wall.

The plasma region Ω can then be described by the mapping,

$$\begin{aligned} r(s, u, v) &= r_0(v) + R(s, u, v) (r_1(u, v) - r_0(v)) , \\ z(s, u, v) &= z_0(v) + R(s, u, v) (z_1(u, v) - z_0(v)) , \end{aligned}$$

where $r = r_1$, $z = z_1$ is the equation of the outer boundary and $r = r_0$, $z = z_0$ is the equation of the magnetic axis. The radial function R satisfies the boundary conditions

$$R(0, u, v) = 0, \quad R(1, u, v) = 1.$$

We also assume that $0 < R_s < \infty$, which implies that the Jacobian is positive and bounded. Let $\epsilon = 1/A$ be the inverse aspect ratio and $K = 1 + \epsilon r$. The magnetic field components are given by

$$\begin{aligned} B_r &= \frac{1}{KD} \left[\frac{\partial(\psi, r)}{\partial(s, u)} - \frac{\partial(\theta, r)}{\partial(v, u)} \right], \\ B_z &= \frac{1}{KD} \left[\frac{\partial(\psi, z)}{\partial(s, u)} - \frac{\partial(\theta, z)}{\partial(v, u)} \right], \quad B_\phi = \frac{\theta_u}{D}, \end{aligned}$$

$$KD = (1 + \epsilon r) \frac{\partial(r, z)}{\partial(s, u)} = \frac{\partial(x, y, z)}{\partial(s, v, u)}$$

where KD is the Jacobian of the mapping.

We now consider the Energy in s, v, u space as a functional of the mapping function R and the potential θ . The first variation can be expressed as

$$\delta E(R, \theta) = - \int [L_1(\theta) \delta \theta + L_2(R) \delta R] ds dv du$$

with the resulting Euler equations

$$L_1(\theta) = \frac{\partial B_2}{\partial u} - \frac{\partial B_3}{\partial v} + L_3(\psi) \psi_\theta = 0,$$

$$L_2(R) = \frac{1}{R_s} [(\theta_v - \psi_s) L_3(\psi) - p'(\psi) KD \theta_v - \left(\frac{\partial B_2}{\partial s} - \frac{\partial B_1}{\partial v} \right) \theta_u] = 0.$$

Here B_1 , B_2 and B_3 are the components of B in the s , v and u directions

$$B_1 = B_r r_s + B_z z_s, B_2 = B_r r_v + B_z z_v + K B_\phi, B_3 = B_r r_u + B_z z_u .$$

The operator $L_3(\psi)$ is related to the first variation of the Energy with respect to ψ ,

$$\delta E(\psi) = - \int L_3(\psi) \delta \psi \, ds dv du ,$$

$$L_3(\psi) = \frac{\partial B_3}{\partial s} - \frac{\partial B_1}{\partial u} - p'(\psi) K D .$$

The Euler equations $L_1(\theta) = 0$, $L_2(R) = 0$ together with the constraints $\nabla \cdot B = 0$, $p = p(\psi)$ are equivalent to the magnetostatics equations

$$\nabla \cdot B = 0 , \, J \times B = 0 , \, J = \nabla \times B .$$

V.- Variational Principle for Island Size

As described above, for any given choice of the poloidal flux function $\psi(s, \theta)$ we can compute a solution to the magnetostatics equations. It is important to determine the poloidal flux function in a self-consistent way, since its properties are crucial in the determination of the confinement properties of a particular solution. The most desirable solutions are those with nested surfaces, since to lowest order charged particles follow magnetic lines, which in turn stay on magnetic surfaces.

In any three dimensional configuration the effect of resonances, corresponding to the small divisors of KAM theory, is the creation of magnetic islands and the resulting deterioration of confinement since particles can be transported across the island through the x points. As the islands grow in size, transport increases and in the extreme case of two large islands overlapping results in total loss due to disruption.

The physical mechanism which is responsible for island growth is resistivity, and it is usually studied using the time dependent resistive MHD equations. This occurs in a much longer time scale than that of ideal MHD and if one wants to compute the time evolution of an island until it reaches saturation it requires a huge amount of computing resources. In practice some simplifying assumptions are usually made by considering a simple geometry, low pressure limit or a reduced set of equations [19].

Instead we propose to compute self-consistent solutions with islands by using a variational formulation which will find the correct island size through an additional energy minimization with respect to perturbations of the poloidal flux function. Boozer has shown that for a perturbation $\delta\psi = f(s)\cos(mu - nv)$ localized in the neighbourhood of a resonant surface $\langle \iota \rangle = \frac{n}{m}$ the change in the energy is negative only in the resistive mode is unstable [16]. Since we allow for finite size perturbations we can compute the saturated island size as a nonlinear bifurcation from the solution without islands.

Let us consider the magnetic field B given by (1) and the poloidal flux function $\psi(s, \theta)$ given by (2 , 3). We minimize the potential energy,

$$E(\psi) = \int \left(\frac{1}{2} B^2 - p \right) dV,$$

subject to the constraints,

$$J \times B = \nabla p, \quad \nabla \cdot B = 0, \quad \int \psi d\theta = \psi_0(s),$$

$$\theta(s, u, v) = u - \frac{nv}{mL} + \theta_p, \quad \psi(s, \theta) = \sum_k \psi_k(s) e^{2\pi i k m \theta}$$

with $\psi_0(s)$ given and $\psi_k(0) = \psi_k(1) = 0$ for $k > 0$.

The Euler equations are obtained from the first variation,

$$\delta \int \left(\frac{1}{2} B^2 - p \right) dV = \int \left(J \cdot \nabla v - p' \right) \delta \psi dV = 0.$$

which leads to the conditions

$$\int \left(J \cdot \nabla v - p' \right) K D e^{2\pi i k m \theta} du dv = 0$$

for all $k > 0$. It is interesting to see what this condition means. As we can show formally, in the presence of a resonance a solution restricted to nested surfaces will have a singular resonant fourier components in the parallel current. As we allow the island to open, this singular behavior disappears when the island reaches its proper size.

The function $\psi_0(s)$ is chosen to correspond to a given average rotational transform $\langle \iota \rangle$ in the case of a Tokamak or it can be computed to satisfy the condition of zero net current in stellarators. The pressure functions requires a little more thought, since in the physical relevant case it must be monotonically decreasing in the radial direction s . The main component of the flux function $\psi_0(s)$ has $\psi'(s_0) = 0$ at the resonant surface $s = s_0$, and it has a minimum there.

For this reason we prescribe $p(\psi)$ to be

$$p(\psi) = P_0 \frac{f(\psi(1)) - f(\psi)}{\int (f(\psi(1)) - f(\psi)) dV}$$

with the function $f(\psi)$ defined as

$$f(\psi) = \pm |\psi - \psi_{edge}|^{XPR}$$

with the minus sign taken if $s < s^-(u, v)$ and the positive sign if $s > s^+(u, v)$, while $f(\psi) = 0$ if $s^- \leq s \leq s^+$ corresponding to constant pressure in the interior of the island.

Here ψ_{edge} is the value of ψ at the edge of the island and the values of $s = s^-$ and $s = s^+$ correspond to the inner and outer edge respectively satisfy the equation,

$$\psi(s^\pm(u, v), u, v) = \psi_{edge} = \psi(s_0, u_0)$$

The resulting function $p(\psi)$ is a continuous decreasing function of s .

VI.- Examples

As we have discussed the BETAS code remarkable accuracy allows us to explore the subtle mathematical behavior of solutions of the variational principle. Figure 1 shows the effect of an $m=2, n=1$ resonance when the flux surfaces are nested. The cross sections of the solution show the crowding of the surfaces around the resonant surface $\iota = 1/2$, with the jacobian of the mapping converging to zero at the X points and converging to infinity at the O points as the mesh size goes to zero, with a clear $m=2, n=1$ dependence. This corresponds to a singular resonant component in the parallel current resulting from the small divisor $(2\iota - 1)$ which is equal to zero at the resonance. Figure 2 shows the resonant component of the mapping function R and the potential θ as a function of the radial coordinate s . The θ component is clearly localized around the resonant surface, and empirical evidence shows that it will approach a delta function as the mesh size goes to zero. The R component has a large gradient at the resonance, with its s derivative related to the jacobian.

As a second example we compare the results from our variational principle for the island size to that of the linear theory of tearing modes of Furth, Rutherford and Selberg [20]. We consider a screw pinch configuration referred as the " Peaked Model ", which is defined by a rotational transform $\iota(r)$ given by

$$\iota(r) = \frac{\iota(0)}{1 + \frac{r^2}{r_0^2}} .$$

Here $\iota(0)$ and r_0 are parameters which determine the stability of the tearing mode. A conducting wall is placed at $r = 1$, and we express the stability results in terms of the parameters

$$x_b = \frac{1}{r_0} , \quad x_s = \frac{r_s}{r_0}$$

with r_s denoting the location of the resonant surface.

For the $m=2, n=1$ tearing mode with $x_b = 1.33$ the results from the linearized theory of Rutherford et al show this mode to be unstable when $x_s < 1.1$ and stable otherwise.

Figure 3 shows the flux surfaces $\psi = \text{constant}$ for the solution of the variational principle in the case $x_b = 1.33$ and $x_s = 0.894$. The linear theory predicts the solution without islands to be unstable in agreement with our calculation. Figure 4 shows the

artificial time evolution of the residuals in the island Euler equation and Figure 5 shows the evolution of the island width for the same case. It is clear that after a suitable time the process has converged and a steady state solution has been achieved. Figure 6 shows the radial structure of the $\cos(3\theta)$ component of the poloidal flux function $\psi(s, \theta)$ when $x_s = 1.09$, an unstable case near the marginal point. Figure 7 shows the two branches of the solution, one corresponding to zero island width and the second branch corresponding to the stable solution with finite island width. The computed bifurcation point can be seen to agree extremely well with the value $x_s = 1.1$ from the linear theory. For $x_s > 1.1$ the variational principle finds the solutions without islands to be stable, also in agreement with linear theory.

As a last example we compute equilibrium solutions for the IMS Stellarator at the University of Wisconsin. It is an $l = 3$ stellarator with 7 field periods. The theoretical design assumes that the toroidal angle dependence is $n = 7k$, with k an integer. In practice however there are error fields with smaller values of n which can resonate and result in island formation. This effects can be studied by simply integrating the equation for magnetic lines in the vacuum field, but it is of practical interest to study what happens to this islands at finite pressure. It should be noted that this is truly a very complicated solution, well beyond the capability and the resolution of any time dependent calculation but very well within the reach of our variational approach.

Figure 8 shows the cross sections of the $s = \text{constant}$ surfaces, with the toroidal shift of the magnetic axis due to the finite pressure. Note that this surfaces are nested, but they are not flux surfaces. In figure 9 the flux surfaces $\psi = \text{constant}$ are shown, with the island structure clearly visible. For comparison with the experiment [21], figure 10 shows experimental measurements of the pressure surfaces exhibiting the same type of islands. The pressure and rotational transform profiles are seen in figure 11 and the resonant components are shown in figure 12. It should be noted that the resonant components of θ and R are quite smooth since the singular current has been eliminated by the island formation.

VII.- The Monte Carlo transport code : A parallel implementation .

It is already clear that the future of massively parallel computing has arrived and that in the immediate future it will be the preferred option for a large class of large scale computational problems.

Because of the completely different computer architecture, a parallel machine requires that we develop new algorithms better suited for this style of computation. Some computational algorithms are by their own nature particularly well suited for a parallel implementation. Among these is the Monte Carlo algorithm for transport calculations in nuclear fusion magnetic confinement devices.

In addition, the transport problem is one of the most important and current topics in fusion research and computational approaches are significantly restricted by the long running times of standard serial algorithms.

Since we have already successfully developed a serial algorithm and computer codes for this problem, relevant questions about the physics and the underlying mathematics have been answered. Thus we only need to change the implementation of the Monte Carlo algorithm to take advantage of its natural parallel features in order to succeed in our objective. It would be far more difficult if we had to explore the mathematics and physics issues at the same time we work on the parallel implementation.

The objective is to calculate neoclassical plasma transport in realistic magnetic confinement configurations. This requires the study of three dimensional effects as well as finite pressure contributions to confinement properties.

The Monte Carlo algorithm [22,8] couples the numerical results of a three dimensional magnetohydrodynamic equilibrium code with particle transport calculations for the drift kinetic equation.

Complicated geometrical and finite pressure effects are included in a numerical solution of the steady state MHD equations,

$$\nabla \cdot B = 0, \quad J \times B = \nabla p, \quad J = \nabla \times B.$$

where B is the magnetic field, J is the current density and p is the fluid pressure. The computer code BETAS includes solutions with non-nested magnetic surfaces (magnetic islands) which had not been explored in previous work. It is also important to note that

the use of flux coordinates and Clebsch potentials for the representation of the magnetic field are important ingredients in the efficiency of the transport algorithm.

The Monte Carlo algorithm can be described as a numerical method of solving the drift kinetic equation of the form

$$f_t + v_d \cdot \nabla_x f = \frac{1}{2} \nu_d \Delta_v f ,$$

where $f = f(x, v, t)$ is the distribution function for the particles, ν_d is the collision frequency, v_d is the guiding center drift velocity and v is the particle velocity. Here ∇_x is the gradient in physical space and Δ_v is the Laplacian operator in velocity space describing Coulomb collisions.

The basic idea of the algorithm is as follows. A particle moves along a drift orbit with a given energy and magnetic moment. After a time interval related to the collision frequency, at some point in space the particle suffers a collision which changes its energy and magnetic moment according to rules given by the collision operator.

We follow a large collection of such particles for many time steps. Simple statistics of the ensemble of particles can be used to estimate functionals of the distribution function f which enable us to compute particle confinement times or transport coefficients.

This procedure can be interpreted as a split time numerical solution of the drift kinetic equation. In the first fractional step, the solution is advanced by integrating along the characteristics (i. e. orbits) of the first order partial differential equation

$$f_t + v_d \cdot \nabla_x f = 0 \quad (1)$$

followed by a second fractional step corresponding to a Monte Carlo solution (random walk) of the diffusion equation

$$f_t = \frac{1}{2} \nu_d \Delta_v f \quad (2)$$

in phase space.

The fact that f is constant along characteristics in (1) is equivalent to particles following trajectories given by the ordinary differential equations

$$\frac{ds}{dt} = v_d \cdot \nabla s, \quad \frac{d\phi}{dt} = v_d \cdot \nabla \phi, \quad \frac{d\psi}{dt} = v_d \cdot \nabla \psi$$

where (s, ϕ, ψ) are flux coordinates in physical space. The drift velocity is given by

$$v_d = \frac{v_{\parallel}}{B} [B + \nabla \times (\rho_{\parallel} B)]$$

with B the solution to the MHD equations, $v_{\parallel}$ the component of the velocity in the direction of the magnetic field and $\rho_{\parallel}$ is the parallel gyroradius

$$\rho_{\parallel} = \frac{M v_{\parallel}}{q B}$$

for a particle with mass M and charge q . For a given particle, energy and magnetic moment conservation determine $v_{\parallel}$ as function of space and allows us to integrate the set of ordinary differential equations for the particle orbits for a prescribed time step.

In the second fractional step, at a fixed point in space, we vary the kinetic energy E and the magnetic moment parameter $\eta = \frac{v_{\parallel}}{v}$ to approximate a solution of the diffusion equation (2). The approximation is a random walk in phase space, where the velocity of the particle moves at each time step δt with equal probabilities to new values given by

$$\eta_{k+1} = (1 - \nu \delta t) \eta_k \pm \sqrt{(1 - \eta_k^2) \nu \delta t}$$

$$E_{k+1} = E_k \pm 2\sqrt{TE_k \nu \delta t} - 2\nu \delta t \left[E_k - \left(\frac{3}{2} + \frac{E_k}{\nu} \frac{d\nu}{dE_k} \right) T \right]$$

where T is the temperature. The sign of the radical is chosen with equal probabilities by a random number generator.

The distribution function f is found to decay exponentially, so we put $f = F e^{-\frac{t}{\tau}}$ with τ the particle confinement time.

We need to take a sufficiently large number of particles and follow them for a long time in order to estimate the value of τ . We compute confinement times for our ensemble of particles from exponential decay of functionals of the distribution function f . A good choice is the expected value

$$\frac{1}{N} \sum_{j=1}^N (1 - s_j) = A e^{-\frac{t}{\tau}}$$

of the radial position s_j of each particle, where $s = 1$ corresponds to the outer boundary. We fit a least square straight line to the logarithm of the functional to estimate the confinement time τ (see fig.13).

Parallel Implementation:

As we have described, The Monte Carlo algorithm requires that we compute particle orbits, energies and magnetic moments as a function of time for a large ensemble of particles. Since all these calculations involve interactions between each particle and the background fields and not between particles, we can distribute the total number of particles equally among the available processors and perform the calculations independent of each other. The only part of the algorithm which requires communication between different processors is the calculation of the functionals of the distribution function and the corresponding decay rate. Since this represents a very small portion of the total computational effort, we expect a large gain relative to serial computation.

CROSS SECTIONS IN PARAMETER SPACE, ASPECT RATIO= 1.00
 MAJOR RADIUS INFINITE MINOR RADIUS= 1.00

Figure 1.- Cross sections showing the effect of a small divisor causing a resonance when the rotational transform equals $1/2$ in a three dimensional solution computed under the restriction of nested flux surfaces. The crowding of the flux surfaces results in the jacobian tending to zero at the X points and the solution develops a singular current. The analytical behavior will be studied in the context of weak solutions.

Figure 2.- Radial dependence of the amplitudes of the resonant Fourier components $\cos R_{21}$ and $\sin \theta_{21}$ for the solution shown in Fig. 1. As the mesh is refined, the R_{21} component becomes steeper at the resonant layer, with its derivative R_r related to the jacobian of the mapping from flux coordinates to physical space. The θ_{21} component is clearly localized around the resonant surface and empirical numerical evidence shows that it will approach a delta function as the mesh size goes to zero.

FLUX SURFACES

Figure 3.- Flux surfaces of a solution obtained with a generalized representation of the magnetic field which allows for solutions with non-nested flux surfaces. Again there is a resonance when the rotational transform equals $1/2$, but instead of a singular current the solutions develop a magnetic island. The amplitude of the $m = 2, n = 1$ island is computed self consistently using a new variational principle for island formation. The equilibrium parameters are $x_s = 0.894$, $x_b = 1.33$.

Figure 4.- Convergence of the iteration to determine the island size is measured by the logarithm of the residual in the Euler equation for the island variational principle. As the plot shows the residual converges to 10^{-10} .

Figure 5.- Evolution of the island size as measured by the island width normalized by the plasma radius for the solution shown in Fig. 3. The converged value for the island width is about 40 percent of the plasma radius. Equilibrium parameters are $x_s = 0.894$, $x_b = 1.33$.

Figure 6.- Radial structure of the amplitude $\psi_1(s)$ of the flux function $\psi(s, \theta) = \psi_0(s) + \psi_1(s) \cos(3\theta)$. The amplitude is very small and it is maximum at the resonant surface. The equilibrium parameters are $x_s = 1.09$, $x_b = 1.33$ which according to the linear theory is very close to the bifurcation point (see Fig. 7).

Figure 7.- Bifurcation diagram showing the two types of computed solutions as a function of the location of the resonant surface x_s . The branch of the solution with island width equal to zero corresponds to the nested case where there is no island present. Linear stability theory of the tearing mode shows this branch to be stable when $x_s > 1.1$ which agrees with the bifurcation point shown in this diagram, and unstable for $x_s < 1.1$. In contrast to the linear theory we can compute the bifurcated solution with finite island size.

CROSS SECTIONS IN PHYSICAL SPACE, ASPECT RATIO= 1.43
 MAJOR RADIUS= 10.00 MINOR RADIUS= 1.00

Figure 8.- Coordinate surfaces $s = \text{const.}$ of an equilibrium solution for the IMS stellarator at the University of Wisconsin. The configuration is an $l=3$ stellarator with 7 field periods, so that in theory the solution has a toroidal angle ϕ dependence of the form $e^{7ik\phi}$ with k an integer.

FLUX SURFACES

Figure 9.- Flux surfaces $\psi = \text{const}$ for a finite pressure equilibrium of the IMS stellarator. Due to error fields the solution is not exactly periodic and lower order resonances with toroidal angle dependence $e^{i\phi}$ give rise to $m = 3, n = 1$ magnetic islands. This type of nonlinear solution with complicated 3D geometry, finite pressure and interaction between long and short wavelengths in the toroidal direction is well beyond the capability of time dependent calculations.

PRESSURE CONTOURS AND VACUUM SURFACE AT 'S' PORT

- Pressure peaks at vertices of triangular surfaces

Figure 10.- Experimental measure of pressure surfaces in the IMS stellarator, showing a qualitative agreement with the computed solutions.

Figure 11.- Pressure and rotational transform in the IMS stellarator. The resonant surface is given by $\iota = 1/3$ and the pressure profile shows a constant value in the island region.

Figure 12.- Resonant components θ_{31} , R_{31} and ψ_1 in the IMS stellarator. The singular current has disappeared due to the island formation resulting in smooth amplitudes $\cos R$ and $\sin \theta$.

Figure 13.- Exponential decay of two functionals of a solution of the drift kinetic equation. The distribution function is computed using the Monte Carlo algorithm based upon numerical solutions of the magnetostatic equations. A least square fit to the logarithm of the functional is used to estimate the confinement time.

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