

Interaction of Flowing Plasma with Collecting Objects

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1 Background

The interaction of plasma with ion-absorbing material objects has been a fundamental problem since plasmas first began to be studied. It has abiding importance because it undergirds the interpretation of Langmuir probes, as well as determining the interaction of space-craft and astrophysical objects with their environment, and the behavior of particle grains in dusty plasmas. The problem is also intellectually challenging because it is inherently non-linear, since the sheath potentials involved are almost always greater than the particle thermal energies. The early work of Langmuir founded the qualitative understanding of the physics, introducing the concept of a sheath when the Debye length (λ_D) is of order the object size (r_p) or smaller [1], and obtaining for symmetric geometries (spherical or cylindrical) approximations based on angular momentum conservation (OML theory) [2] that give essentially exact results for flux when $\lambda_D > r_p$. Bohm's identification of the necessary minimum ion velocity entering the sheath [3] was an important further insight, and eventually a rigorous formulation of the collisionless problem by Bernstein and Rabinowitz [4] was solved numerically with Maxwellian ion distribution by Laframboise[5, 6], for a wide range of relevant parameters. Asymptotic matching of approximations to the solutions across the sheath boundary has remained for many years a mathematical problem of interest (e.g. [7]), often poorly understood by non-expert authors. The classic solutions are of the symmetric (flow-free) and collisionless situation. In the 1960s and 70s substantial attention was also paid to the situation of flow. This was primarily motivated by the question of the interactions and notably the wakes of satellites in space plasmas[8]. Satellites are most often moving at supersonic speeds with

respect to the plasma. These theoretical studies mostly used various forms of linearization of the plasma response [9, 10] which, while convenient, are of questionable accuracy. Some early attempts at more complete particle-orbit based calculations generally did not account for the self-consistent potential variations, notably potential asymmetries [11, 12]. Because of the unknown accuracy of these approximations, and their known inaccuracy close to the object, the flowing plasma problem remained until recently a vexed and unresolved problem.

Attention during the last decades of the twentieth century also turned to the effects of collisions, which appeared to be responsible for the significant discrepancies that many experiments observed when compared with the collisionless theories. Studies in recent years have reemphasized the ability of even very rare collisions to populate trapped orbits and thus influence the shielding [13].

The need for definitive solutions of the interaction of a flowing plasma with an object became increasingly pressing as more widespread experimental implementations of Mach probes occurred. In magnetized plasmas (ion Larmor radius $\rho_i \ll r_p$) persuasive theoretical analysis for their parallel calibration (the relationship between upstream to downstream flux and parallel Mach number) was established [14, 15], but in unmagnetized plasmas, no such theory existed [16]. The development, by the present author, of the Specialized-Coordinate Electrostatic Particle and Thermals in Cell (SCEPTIC) code [17–19] was initially motivated by need for this calibration for unmagnetized Mach probes, but it has proven of far wider significance. An NSF/DOE basic plasma grant has enabled the exploitation and further development of this research through partial support of a Research Assistantship for a graduate student to work on the project. The present proposal is for a renewal of support for ongoing and new studies in this important and intellectually rich research area.

2 Findings

The proposer’s computational flowing plasma group, supported in part by NSF/DOE since 2006, has been enormously productive. It has published 22 journal articles, of which 3 are in Physical Review Letters; received a total of 330 citations, and made 5 invited and numerous contributed presentations at international conferences. In addition, other groups have published at least 3 papers [20–22] based upon results they have obtained from the SCEPTIC code, developed by the proposer. The codes developed for this subject are Particle In Cell (PIC) codes, representing the entire ion distribution function and its variation in space in the vicinity of an absorbing object.

Under this grant, the research proposed in 2009 consisted of four research topics, under whose headings the recent scientific findings and achievements are briefly explained.

2.1 Exploitation of SCEPTIC3D to understand probes and grains in turbulent plasma.

The 3-D version of SCEPTIC (actually 6-D in phase space: 3-D, 3-v), has been used to explore the interaction of a spherical object with collisionless flowing plasma over the whole

spread of the important controlling parameters. Those are the dimensionless ratios of (i) the Debye length λ_{De} , and (ii) the Larmor radius ρ_i , to the object size; and (iii) the electron to ion temperature ratio T_e/T_i . This was the doctoral project of Leonardo Patacchini.

Some highlights of this work are: excellent confirmation[23] of the recent analytic theory[24–26] of transverse Mach probe operation, in the strong-magnetic-field limit, which provides new insight into how Langmuir probes really work in magnetized plasmas; provision of validated calibration factors for Mach probes; comprehensive evaluations of how the ion current varies with magnetic field strength.

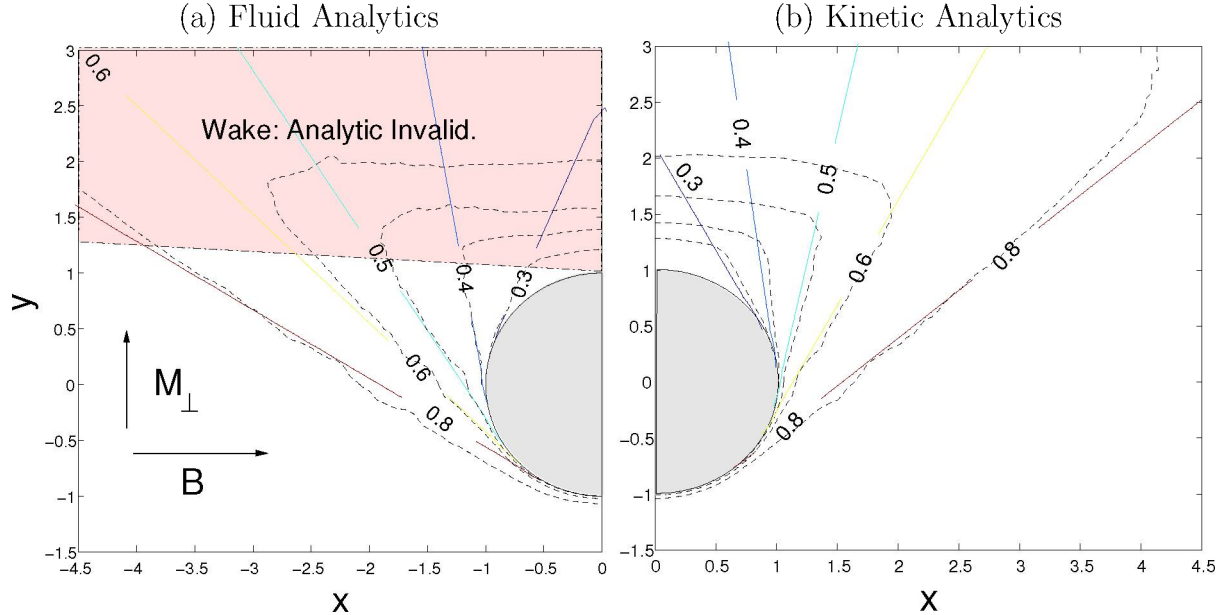


Figure 1: Examples of excellent agreement of density (n/n_∞) contours in the region of validity of analytic ($r_p/\rho_i = \infty$) (solid) and SCEPTIC ($r_p/\rho_i = 20$) (dashed) solutions. (a) $T_i/T_e = 0.1$, $M_\perp = 0.5$, fluid analytic values; (b) $T_i/T_e = 1$, $M_\perp = 1$, kinetic analytic values.

Studies of the effects of finite Debye length[27] observe that when the Debye length exceeds the Larmor radius, an important transition occurs, because the sphere starts to shield the convective electric field driving the cross-field flow. In this regime, the ion collection can exceed the unmagnetized OML value.

Comprehensive studies of the forces on a spherical particle in $E \times B$ plasma flow[28] over the range of possible Debye lengths and Larmor radii indicate that the forces arising from internal currents in a conducting particle will cause it to gyrate faster than would be implied by its charge to mass ratio. Moreover when the Debye length is large, the code calculation shows that the transverse ion drag can become “negative” (i.e. in the direction opposite to flow) but the other forces always overwhelm it, so that spontaneous motion does not occur.

2.2 Inclusion of additional particle species.

This work envisaged the addition of the dynamics of species such as neutral atoms or electrons to the particles moved by the PIC code processes. (Electrons in the hybrid codes we have been using are by default treated as a light fluid governed by a Boltzmann factor.) This is the area of research taken up by the current doctoral student Christian Haakonsen.

First, in his Masters dissertation, Haakonsen implemented charge-exchange collisions within SCEPTIC3D. Although collisions had already been implemented in the 2-D version of SCEPTIC, where drift velocity can only be parallel to any magnetic field, the 3-D work of Patacchini had focussed on oblique flows in *collisionless* plasmas and left aside the issue of collisional cross-field flow. Subsequently SCEPTIC3D was modified to allow for charge-exchange collisions. This required the development of a new scheme for particle injection at the outer boundary, since the previously implemented scheme of injecting particles according to a drifting Maxwellian distribution no longer applied. The new scheme incorporates a Monte-Carlo approach to calculate the modified distribution function, accounting for charge-exchange collisions, neutral drift, and external applied electric field.

This new capability (and a number of other improvements to SCEPTIC3D) was benchmarked in appropriate cases against SCEPTIC results and then used to explore the collisional enhancement of ion flux to a sphere *when the plasma is flowing*, resulting in a well-received presentation at the International Conference on the Physics of Dusty Plasmas[29]. Magnetized plasmas were investigated and found, somewhat surprisingly, to experience an increased ion current enhancement by collisions.

For his Doctoral research, Haakonsen has undertaken to develop a code that is capable of accommodating arbitrary external distributions of ions *and* electrons. This code will take advantage of the fact that for most purposes the plasma flows we are studying are stationary. [There are some important cases in which one expects the distribution functions in the surrounding plasma to be unstable to electrostatic waves and hence non-stationary; but these are challenging to capture in a global simulation; see later, section ??.] The challenge involved in including electron kinetic modelling via Particle in Cell treatment, is that it forces a far shorter timestep to resolve the *electron* plasma period, rather than simply the ion plasma period for the hybrid approach of SCEPTIC. To avoid this greatly increased cost, the new code will bypass all the time-dependency and approach the problem in a different (not PIC) manner. Instead of tracking orbits forward in time, the ion and electron densities will be determined by tracking orbits backward from the density location until the external plasma (or a bounding surface or a collision) is encountered. This can be done either in a prescribed (e.g. precalculated) potential, or by an iterative approach in a self-consistent potential. The full ion and electron distributions are thereby calculated with approximately equal numerical effort, on the chosen mesh.

The code, the “Plasma–Object Simulator with Iterated Trajectories” (POSIT), works with an unstructured 3-D spatial mesh (of tetrahedra) by leveraging an implementation of the iMesh interface from the DOE Interoperable Technologies for Advanced Petascale Simulations center[30]. Using an unstructured mesh provides great flexibility in the shape of the computational domain and of any collecting objects or surfaces (of which there can be any

number). Further, the use of the iMesh interface enables visualization of the results using standard tools such as VisIt[31], avoiding any need to invest effort in developing custom visualization tools. At present POSIT can treat electrons and ions in a quasineutral plasma, and its unmagnetized operation has been benchmarked against analytic results using a spherical object and domain. Magnetized orbits have been also implemented, but operation in this mode remains to be fully benchmarked against SCEPTIC3D.

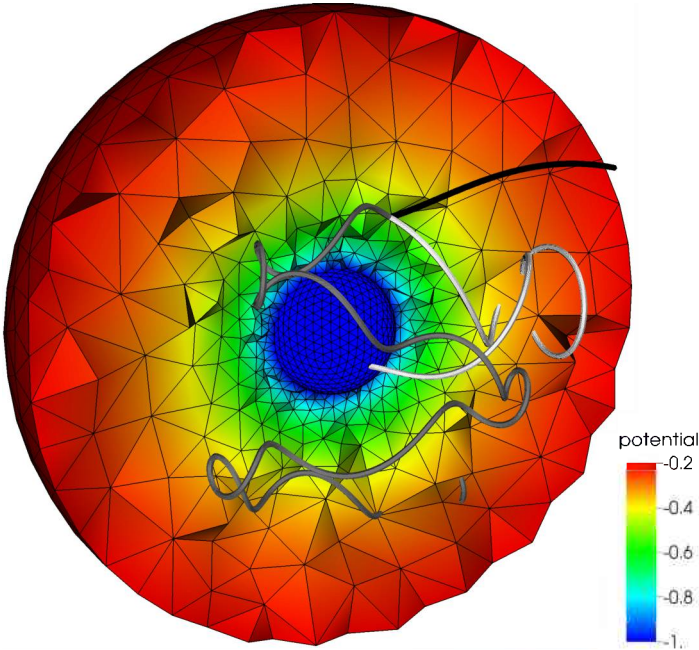


Figure 2: Representation of potential near a sphere with POSIT’s unstructured mesh, displayed using the VisIt package. Three types of ion orbit arising in the combined electric and magnetic fields are illustrated. The orbits, all tracked back from the same point of interest, can be “finite” terminating on the sphere (light gray); “infinite” extending to infinity (black); and “trapped” (dark grey).

The ability to evaluate the velocity distribution of any species at any point in the domain makes POSIT a powerful tool for exploring the validity of assumptions built into codes such as SCEPTIC3D. For example, the electron current to an object at floating potential in a magnetized plasma can readily be calculated based on the potential structure from SCEPTIC3D, as can the sensitivity of the ion distribution function to collisions, etc.

2.3 Interaction with cylindrical objects.

The special coordinate system in SCEPTIC is spherical, which enables it to solve problems involving a sphere with great accuracy at moderate cost. It was envisaged that it would be worth developing an alternative version of the code which employed cylindrical coordinates, and this would have been a valuable tool for cylindrical studies. However, it proved possible to use some of the more general tools that were being developed, to address the cylindrical scientific topics of most interest. Therefore specifically cylindrical code development has been postponed indefinitely in favor of using POSIT and the newly developed 3-D code COPTIC, described next.

2.4 Calculations of wake and multiple-object interactions.

A plasma wake behind an object can extend in some cases very many object radii. That makes it rather inefficient to use a spherical coordinate system centered on the spherical object to calculate the wake. A cartesian coordinate mesh is more appropriate. Moreover, some of the most interesting problems in dusty plasmas involve not a single isolated dust grain but several (sometimes many) grains, which interact with one-another's wakes. A system with more than one object in a flowing plasma typically has *no* even approximate axis of symmetry; so one must do a 3-D calculation and it might as well be cartesian, but it must be able to accommodate object surfaces oblique to the mesh coordinates. These simple ideas are what motivated the development of the Cartesian-coordinate, Oblique-boundary, Particles and Thermals In Cell, or COPTIC code.

This has been a programming project of the proposer (without substantial student involvement yet) for several years. COPTIC is (like SCEPTIC) a hybrid PIC code. It has a cartesian mesh of cells (though not necessarily uniformly spaced). Bounding surfaces (e.g. equipotentials for a conducting object), whether planar or curved, can intersect the node lattice at any angle. The difference stencil by which Poisson's equation is represented (and solved) is adjusted for the presence of boundaries in such a manner as to maintain second order accuracy in the solution for the potential, and in its interpolation to obtain the electric field at any intermediate point[32]. This avoids the extremely crude "stairstep" representation that is often used for oblique surfaces on cartesian meshes. The objects in the code are represented by a few important shapes (spheres, cylinders, cuboids, parallelopipeds, etc) and their sums or differences. The generality of this approach has required considerable development investment in such geometrical challenges as determining at high speed which of various disjoint volumes an ion might be in, or determining the distribution of ion flux over the surface of these different objects. The code is still under development, but is already in an excellent state of verification, validation and productivity. It is fully parallelized for running on MPI clusters, and it runs extremely fast. Production runs with hundreds of millions of particles are routinely completed in a wall-clock time of an hour or two. Three journal articles have already been published based upon its results.

The wake of a single small particle has been studied using COPTIC[33]. An example is illustrated in Fig. 3. At very small (normalized) particle size and charge, results show excellent agreement with the (few) reliable published Linear Response formalism calculations. However, since COPTIC does a fully non-linear calculation it is able to study larger particles (and hence larger charges) and to show where non-linearity becomes important and changes the wake. These studies have corrected erroneous pictures of the form of the wake, helped to explain such phenomena as oblique alignment of particles floating in discharge sheaths, and established that non-linearity becomes important even for rather small particle size threshold $r_p/\lambda_{De} \sim 0.01(v_d/c_s)^2$, relevant for many dusty plasma experiments, especially when the plasma drift velocity (v_d) is small compared with the sound speed (c_s).

Two-particle calculations have been performed[34] and, for the first time ever, the full resulting interaction force has been obtained rigorously from code calculations. The result

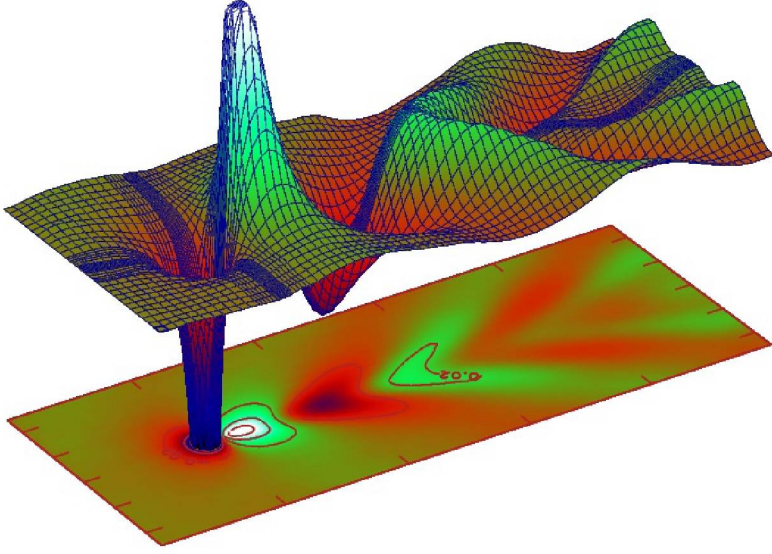


Figure 3: Example of the potential trailing a small particle in a plasma flow of Mach 1, sliced along a plane. The negatively charged particle causes a deep potential well at its position, but ion focussing then forms a positive peak trailing the particle. Subsequent oscillations give the impression here of a water wake, although its wavefronts are actually 3-D cones. The wake damping depends on collisions, temperature ratio, and non-linearity.

shows that contrary to some prior claims[35] the transverse (particle chain-forming) force is very well represented by the gradient of the upstream-grain's wake at the downstream-grain's position. This despite the non-linearity (also established by COPTIC) of the single particle wake. More recently[36] these results have been extended to lower Mach numbers, showing the vanishing of the grain aligning forces below approximately $v_d/c_s \sim 0.3$ (a result that is due to non-linearity, and hence not observed by Linear Response calculations).

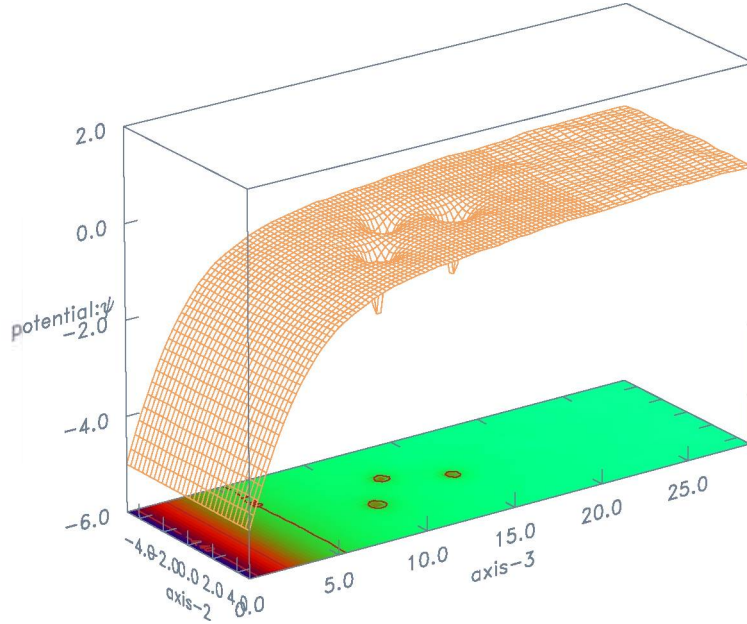


Figure 4: Three particles floating in a sheath simulated by COPTIC. A slice through the 3-D simulation of the potential is plotted, over part of the domain of this initial scoping exploration. The small particles produce local minima in the potential. The overall potential gradient into the sheath is produced by the boundary conditions. Units of length are λ_{De} ; units of potential are T_e/e .

The capability of COPTIC to address non-uniform plasmas and multiple objects is illustrated in Fig. 4.

2.5 GPU implementation of SCEPTIC3D

Because Christian Haakonsen won a fellowship, it was possible to support a second graduate student, Josh Payne, for a one-year Masters project. We decided to tackle an interesting problem beyond the original scope of the grant. The project consisted of porting SCEPTIC3D to run on a graphical processing unit (GPU), using the CUDA coding architecture. This was a ridiculously ambitious project for such a short duration. However, Payne was already established (through undergraduate research with the proposer) as an expert in GPU programming; and fall-back dissertation achievement targets were possible if the challenge were to prove too great. In the event, they were unnecessary. Payne completed the port and was able to do extensive benchmarking of speed and correctness relatively comfortably[37]. This was an outstanding achievement because it required, in addition to identification of optimal sorting approaches and development of new parallelism algorithms, extensive restructuring of the code to separate out the parts to be carried out on the GPU, and hand optimization of the GPU code implementation. It is well known that PIC codes do not benefit very much from GPU parallel processing capability unless they are specifically [re]written to take advantage of GPU strengths (raw computational power) and avoid their weaknesses (limited fast memory-access size). We discovered that many of the published approaches to solving this problem are highly complex and specific, while not always producing the fastest results. Instead we were able to use CUDA Thrust library standard sorting packages to produce an integrated code that overall runs roughly 70 times faster on a GPU than it does on a single CPU. This code (like our others) is available publically for anyone to use. Because we have access to a parallel cluster of 600 CPUs, but not to one with large numbers of GPUs, the GPU capability does not substantially enhance our local research opportunities. However, it makes the code more powerful for others who do not have access to a big CPU cluster but do have a GPU. It also prepares SCEPTIC3D for more massively parallel operation on multi-GPU forefront computing installations. Moreover, this work has established some important programming solutions for PIC codes generally.

3 Broader Impacts

The primary costs of this project are to support a graduate student's education. Thus the integration of education and research is integral to the proposal. Moreover the MIT Plasma Science and Fusion Center has an active outreach program that involves a dozen or more middle- and high-schools per year visiting to hear introductory talks and view the experiments. The proposer and his graduate students are active in such outreach events which help to inspire K-12 students with the excitement of the STEM fields, and specifically plasma physics. Christian Haakonsen took top graduate-student-prize for outreach last year.

Because the topics to addressed in this project arise in the simplest of plasma diagnostics and in dusty plasmas that can be produced experimentally with only rather modest equipment, these are aspects of the plasma field that connect to efforts in some of the less prominent educational institutions, some of which are notable for their minority faculty and

students.

A major contribution to enhance research infrastructure is the development of the large-scale computer codes by this project. Scientific software is at least as important as scientific computing hardware. The portability of the codes is an important feature that enables the proposer to make them freely available for download on the internet. The present release versions are already available on github[<http://github.com/ihutch/>]. We have given direct assistance and advice to several groups on how to run the released codes, and several groups have profitably done so.

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