3-D DSMC Simulations of Comet 67P/Churyumov-Gerasimenko. Y. Liao[1], C.C. Su[2], S. Finklenburg[1], M. Rubin[1], W.-H. Ip[3], H.U. Keller[4], J. Knollenberg[5], E. Kührt[5], L.-I. Lai[3], Y. Skorov[4], N. Thomas[1], J.-S. Wu[2], Y.S. Chen[6].
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Introduction: As the development of ESA's Rosetta mission started, it became clear that the physics of the outflow immediately above the surface needed to be understood. Low production cases needed to be investigated for comparison with observations at high heliocentric distances. In these cases, the fluid assumptions begin to break down. In particular, ice sublimating into vacuum forms a non-equilibrium boundary layer, the "Knudsen layer" (Kn-layer), with a scale height of ~20 mean free paths (mfp) [1,2]. If the production rate is low, the Knudsen layer does not relax in an equilibrium region but goes directly into a region with non-equilibrium gas because of expansion. The velocity distribution function (VDF) is strongly non-Maxwellian. The production rate of H_2O gas varies strongly with heliocentric distance. When Rosetta encounters comet Churyumov-Gerasimenko (C-G), the mfp will be of the order of metres (localized outgassing) to kilometres (homogeneous outgassing) [3,4].

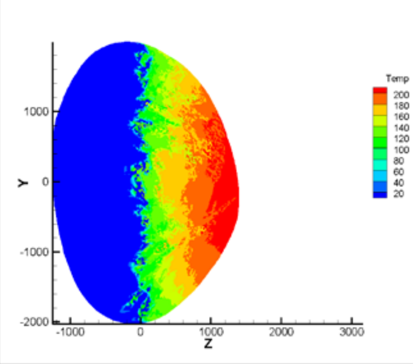

Figure 1 The 3D-shape model of C-G has been imported into the code. A temperature for the surface at 3.25 AU has been calculated from the surface energy balance (neglecting heat conduction) and has been overlaid. The Sun is in the +z direction. The axes are in metres.

The state-of-the-art method to study gas flows inside non-equilibrium regions is the Direct Simulation Monte Carlo (DSMC) [5]. The basic idea of this technique is to represent many real gas molecules by a few model particles and apply statistical collision models to them. The gas parameters (density, velocity, temperatures) are obtained by averaging the properties of the particles in sampling cells. Pioneering work on the use of DSMC for cometary applications has been performed by [6,4] and several other authors have also worked on this topic. Comparisons between DSMC and fluid techniques have also been performed to establish the limits of these techniques [6,7].

The drawback with 3D DSMC is that it is computationally highly intensive and thus requires the use of powerful computer clusters. However, the structure of the algorithm allows parallel computing on Graphic Processor Units (GPUs) [8] to increase performance dramatically. We are currently working towards implementing a cometary application on GPUs but have started with the conventional CPU approach using a dedicated 32 node cluster. We have already studied a case with comet 9P/Tempel 1 where the Deep Impact observations were used to define the shape of the nucleus and the outflow was modelled in an attempt to fit the observations of water emissions at 2.66 micron [9,10]. Here we report on some preparatory models of the outflow from the Rosetta target, comet 67P/Churyumov-Gerasimenko (C-G). Our aims are to (1) determine the gas flow-field in the innermost coma, (2) determine the surface outgassing properties from analysis of the flow-field, (3) determine initial velocity, bulk composition, and surface fluxes, (4) investigate dust acceleration by gas drag and (5) compare with observations over a range of heliocentric distance.

Boundary conditions: The calculations have been performed using the nucleus shape model of [11]. The model has a surface area of 30.63 km^2. Models have been run at several heliocentric distances. A surface temperature has been defined which is shown in Figure 1 for the case at 3.25 AU.

The DSMC program used is $PDSC^{++}$ [12] which is based on the PDSC code developed by Wu and coworkers [13-15]. $PDSC^{++}$ allows a parallel simulation of 2D, 2D-axisymmetric, and 3D flows on hybrid unstructured grids. The unstructured grid has been defined with the help of "Gridgen" before the DSMC simulation is started. The typical cell dimension is 3.8 m on the nightside and 2.8 m for the dayside (comparable to the Rosetta camera resolution from 150 km). 761592 cells were used. The domain extends out to 10 km from the centre of the nucleus. A variable timestep and a transient adaptive sub-cell technique have been used to increase computational speed and accuracy in regions of high density. Parallel performance is optimized by use of a domain re-decomposition method. A half-Maxwellian VDF at the surface temperature is used to initialize the gas outflow from the surface. Although different species have been simulated we concentrate here on water vapour and use standard values for the collision model.

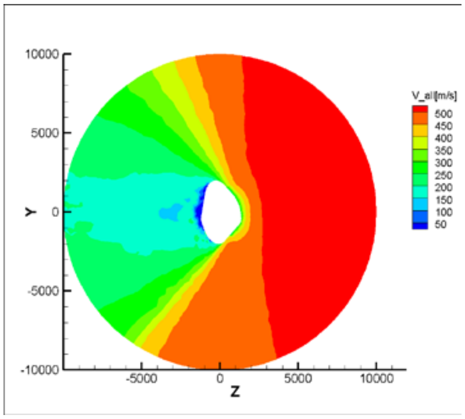

Figure 2 The gas velocity in the x-z plane of the 3D model of outflow from C-G at 3.25 AU.

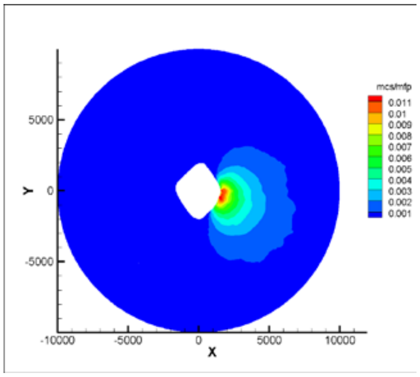

Figure 3 Mean collision separation/mean free path for the model. This plot shows that the calculation gives an mcs/mfp of less than 1 which is desirable for a valid DSMC calculation [5].

Results: Figure 2 shows the velocity of the outflow from the C-G simulated at a heliocentric distance of 3.25 AU with a production rate of 10^{24} molecule s^{-1}. Emission is restricted to the dayside hemisphere by the temperature which controls the emission rate. Outgassing from the sub-solar point is dominant.

There are several points to note. Firstly, there are some numerical artefacts evident, particularly above the nightside (to the left) where densities are low, indicating that additional simulation molecules would improve the solution. Secondly, the expansion towards the nightside seen in early fluid dynamics calculations at higher densities (e.g. [16,17]) is clearly evident. Thirdly, the velocity is quite similar to the homogeneous spherical nucleus model of [18] although the production rate used there was around a factor of 60 higher. The nucleus model is based on ground-based and HST observations and is therefore of low resolution. However, the 3D shape does break the symmetry.

In Figure 3, we show the mean collision separation/mean free path ratio. This should be <1 to provide good results [5] and this is seen to be the case through the flow field even at the centre of highest activity.

Conclusions: Our DSMC code (PDSC^{++}) has been used to study a variety of simple models of the gas outflow from comet C-G. The code uses an unstructured grid and can provide global values for gas density, velocity and temperature out to 10 km from the nucleus at resolutions of better than 10 m within 24 hours on a 32 core parallel machine. Predictions for the flow velocity at 3.25 AU under simplified boundary conditions have been presented.

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