Executive Summaries

A brief description of each problem is given followed by the equation-free Executive Summary for the problem

OPTIMIZATION OF DELIVERIES FROM DISTRIBUTION POINTS

CaterPlus

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Description

- The problem that the Study Group was asked to investigate involves the distribution of food and household items. There is a large area containing customers and each customer has a unique demand for a product that is being delivered. The company wants to organise delivery by splitting the customer base into smaller regional units served by distribution points. Each distribution point has some transportation capacity to deliver products to the customer. The problem is to find the location of these distribution points and to organise the transportation capacity to deliver products fulfilling the demands of every customer. The total transportation capacity is determined by the fixed number of trucks. The goal is to minimise the cost of delivery.

Executive summary

- This large problem was found to be outside the scope of the Study Group. The Study Group investigated the simpler problem of only one fixed distribution point from which all trucks operate. The solution was viewed as a combination of two separate processes. In the first part customers are clustered into groups whose demand can be served by the capacity of one truck. The second part is to solve for optimal cost for each single truck route. An approximate algorithm was implemented in which customers are sorted by their demand. The algorithm may also be useful for the more general problem of more than one distribution point.

ANALYSIS OF THE POTENTIAL MECHANISMS OF ROCKBURSTS

Gold and Platinum Mining Industry

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Description

- The occurrence of so-called "rockbursts" in deep level mining operations is of continuing concern to the South African mining industry in being a potential cause of serious injuries to miners and in curtailing the exploitation of valuable mineral resources. Surface tremors may, in extreme cases, even cause damage to buildings or other infrastructure. Understanding some of the underlying deformation mechanisms of rockbrusts can clearly have considerable benefits in devising engineering strategies to ameliorate the potential damage and safety risks of deep level mining. Three main areas of potential interest are:

  a) *Prediction*: Precursory signals of seismic activity or other changes may be used to infer the impending onset of large seismic events.

  b) *Excavation damage*: An improved understanding of wave propagation effects, initiated by sudden rock failure, can be used to design improved support systems in underground excavations.

  c) *Localisation theory*: Further advances in understanding the intrinsic structure of rock failure mechanisms can assist in the assessment of the likelihood of rock failure in the vicinity of existing excavations.

Executive summary

- During the MISG study week efforts were concentrated on formulating a simple model to address the first area of interest, relating to the prediction of a seismic event. In order to fix some ideas a basic fault creep model was analysed. The objective was to determine whether this model would display an initial "slow" slip behaviour (precursory phase), followed by a rapid acceleration of fault slip ("rockburst"). It was assumed that slip movements on the fault were proportional to the difference between the total shear stress acting across the fault and the overall resistance to fault slip, comprising both cohesion and sliding friction components. The further assumption was made that the cohesion decreases as a linear function of the progressive slip across the fault. Using a complex variable displacement discontinuity boundary integral approach and some specific assumptions relating to the shear stress loading profile, it was found that the fault movement could be described in terms of a single non-linear ordinary differential equation. This differential equation can be expressed in terms of dimensionless variables, B and T, representing the active length of the fault and the time respectively. In the particular case that was studied, the differential equation was shown to contain a dimensionless parameter group, comprising the elastic shear modulus, the cohesion weakening slope parameter, load profile constants and the slip rate proportionality factor. The equation is also dependent on the host material Poisson's ratio. A preliminary numerical analysis of this equation showed that the activated crack length would initially extend at a decreasing rate and then accelerate exponentially agreeing qualitatively with the conceptual model of some "incubation" phase followed by rapid movement. Further explorations of the properties of this equation and other slip resistance models are required.

HIV MODELLING IN A LABOUR FORCE

Mining Industry

Industry Representatives
Two medical practitioners from the sector

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Description

- The problem that was presented to the Study Group pertained to workers who had been diagnosed to be HIV+ and were participating in a wellness programme.

  The Study Group was asked to analyse available workers' demographic and clinical information, spanning a period of five years. The aim of the investigation was to determine indicators that could be used to predict whether or not a given worker who has been diagnosed to be HIV+ and is currently participating in the wellness programme will return to work. Further to this, if there were indicators as to whether the worker will return to the same job category and what was the probability that the worker would be placed on that particular job for some time in the future.

  The Study Group had access to a sample of a clinical database of the workers, only identifiable by an index number. The data collected for each patient were those of certain clinical and physical characteristics measured at different points in time by medical staff.

Executive summary

- The Study Group identified some models that could be suitable to answer various aspects of the questions posed. One of the models was the Classification and Regression Tree Analysis (CART) model which is used widely in the development of clinical decision rules. This technique is also able to uncover the interaction between the variables contained in the dataset.

  Another proposed approach was the use of life tables to compute the probabilities that workers would survive different time periods into the future. Both approaches required that the data be re-organised through the use of data mining techniques. The Study Group used off the shelf CART software and were able to determine some prominent variables that are usable as indicators for placement to the various job categories. The life tables model requires the development of custom software to automate the laborious process.

On the question of forecasting whether a worker would remain in the same job category for a certain length of time, the Logistic Regression Model was applied to the dataset. This model also highlights certain variables as prominent for different time periods and seems to suggest some interesting results from further application of the model would be realised. It was also able to highlight some varied degree of association between the variables.

The results obtained from the few experiments on the sample data are encouraging and need to be verified against a larger dataset. The group intends to run more experiments and investigate the usefulness of the software further.

MODELLING TEMPERATURE, MOISTURE CONTENT AND MATURITY IN CONCRETE DAMS

Cement and Concrete Institute

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Description

- At the first Mathematics in Industry Study Group meeting in 2004, a mathematical model was developed to analyse the temperature, moisture content and maturity in concrete dams. Maturity describes the degree of hydration which occurs when water and cement are combined. By considering heat conservation, hydration chemistry and water conservation, three coupled nonlinear partial differential equations for the temperature, moisture content and maturity were derived. Since the moisture diffusivity of concrete depends on the moisture content, the moisture content satisfies a nonlinear diffusion equation. The Study Group was asked to investigate analytical and numerical solutions of this system of equations subject to suitable boundary and initial conditions for models of hydration of concrete dams.

Executive summary

- The starting point for our analysis was the set of equations derived at MISG 2004. In that work a set of three equations describing the temperature, maturity and moisture content were set out, together with appropriate boundary conditions. Our first goal was to remove some of the restrictions and simplifications employed in this initial investigation.

  Perhaps the most apparent simplification employed was to set the temperature at the surface of the concrete to the ambient temperature. However, it is common knowledge that materials do not conform to the surrounding temperature, which is why, for example, hot air can be seen rising from a road on a hot day. The road is clearly hotter than the surrounding air and so transfers heat to the nearby air. We replaced the

previous boundary condition with a standard cooling condition (or Newton cooling condition). The condition allowed heat transfer between the concrete and surrounding air and included a source term to represent solar radiation. In fact this condition had also been derived by a separate group at MISG 2004.

Our second major change was the source term in the heat equation. Previously it had been set as proportional to the rate of change of moisture. In fact the source term is the rate of change of heat generation. Graphs presented during the meeting indicated that the relation between the two quantities was far from linear and hence the true heat generation term must be employed.

A final change was to the symmetry conditions applied at the centre of the block. Whenever the block is laid, the bottom surface will be subject to different conditions to the top. For example, it will not be subject to solar radiation or convective heat transfer from the air, the evaporation will also be different due to the different temperature and air flow. It will either sit on a lower block or the building foundation and is therefore most likely to lose heat by conduction. Symmetry at the centre is therefore clearly inappropriate. Given our lack of knowledge of the base we first assumed the lower surface to be insulated and then replaced this assumption with a cooling condition. We also assumed that no moisture was lost at the bottom; this could easily be changed.

Our first task with the new equations was to non-dimensionalize them. This highlighted a number of small parameters, and so indicated the dominant effects in the process. Small parameters in front of the diffusion terms in both the moisture and heat equations indicated that there would be thermal and moisture boundary layers near the block surface. A small parameter in the maturity equation indicated that, under certain parameter regimes, the temperature effect on maturity would be relatively small.

Neglecting all small terms in the non-dimensional system allowed us to find an approximate bulk solution. Taking the variation of heat generation with maturity as piecewise linear, i.e. the sum of two linear parts (which seemed a reasonable first approximation to the bell shape that was presented), we found that the water content decreased linearly with maturity. Temperature was approximately quadratic in maturity and the maturity produced a solution in terms of two exponentials. In particular the solution depended critically upon a parameter denoted by α_7 (note, α_7 is the ratio of the stoichiometric ratio for the hydration reaction and the initial moisture content, so it should be an indicator of how far the reaction is likely to go). If $\alpha_7 \leq 1$ then the maturity increased exponentially with an asymptote at $m = 1$, i.e. the reaction will be complete in infinite time, but for practical purposes the reaction is almost complete (not noticeable) at finite time. However, for $\alpha_7 > 1$ the increase is again exponential, but this time the asymptote is $1/\alpha_7$, i.e. the reaction will never be complete. This is consistent with the moisture solution which shows that when $m \to 1/\alpha_7$ the moisture $\theta \to 0$. So the water runs out before the reaction is complete. It is also consistent with experimental data.

A numerical solution was also presented to the coupled thermal moisture equations, using a more realistic energy source term $Q \sim me^{-\beta m}$. The dimensionless equations were semidiscretised in space using centered-differences, and then solved using an ODE solver in Octave. Simulations run with a value of $\beta = 8$ (which gave a qualitative function for Q similar to the bell-shaped function that was presented), showed that the exposed surface of the concrete was at a higher temperature initially, and that the slab was heated from top to bottom until a uniform temperature was achieved throughout the slab for later times.

Finally, a numerical solution to the full system was presented. The three equations were discretised using a partially implicit numerical scheme. Simulations were conducted for a two month period with different building scenarios for a six meter thick concrete layer.

POLAR PLOTS OF DIAMOND SURFACE ENERGY

Mining Industry

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Description

- The manufacture of synthetic diamonds produces crystals in a variety of habits, such as cubic, octahedral and mixed habit. In all cases the basic structure of the crystal is the unique diamond lattice, and the various habits arise from differences in the orientation of the faces of the crystal relative to the lattice. It is well understood that the surface energy of the different orientations is what determines which face types grow during manufacture. Polar plots are a way of plotting surface energy in orientation space, and allows one to compare the energy of two face orientations and all intermediate orientations formed by linear combination of the two orientations. The surface energy can be shown on a polar plot: the radius is proportional to the energy, and the polar angle gives the degree of mixing between the two face orientations.

  It turns out that the polar plot has some very sharp local minima, which play a very big role in determining what type of crystal is grown. MISGSA 2006 was presented with a paper (Terentiev 1999) apparently describing the polar plot for any two orientations, and the task was firstly to understand the paper, and secondly to analyse it for correctness.

Executive summary

- Terentiev's formula for vacuum surface energy is correct only in an average sense, and gives an artificially smooth polar plot. It fails to predict the very sharp local minima associated with some of the orientations. As these minima are the most influential in the crystal growth, this formula cannot be used to model what really happens during diamond manufacture.

  We were able to calculate vacuum surface energy directly, using a simple geometric approach to counting the "bonds" (which are not real bonds but rather the unfilled bond orbitals of the carbon atoms forming the surface). This completely solves the problem as initially stated. However, this is limited to a case-by-case calculation, the complexity of which is proportional to the number of fundamental diamond lattice units required to describe the orientation, and therefore can only approximate a polar plot of vacuum surface energy by means of a set of discrete points.

We suggest that the local minima of the polar plot arises from the simple cases fully described by using a small number of lattice units, and that for an orientation requiring a large number of lattice units the surface energy is very close to that of the smoothed value given by Terentiev's formula. Thus a good approximation to a polar plot would be to calculate exactly the surface energy for those linear combinations that require a small number of lattice units and to interpolate intermediate values by means of Terentiev's formula.

We made some progress towards understanding non-vacuum surface energy, that is, the energy of the interface between an immersed crystal and a fluid. In this case, the bond orbitals of the surface atoms interact with the fluid at atomic scales. The paper gave results of an incompletely described simulation, and we made some progress towards reproducing similar results. This appears to hold some promise for modelling the process of diamond syntheses, and a version of these simulations will be included in the report.

References

Terentiev, A. Molucular-dynamics simulation of the effect of temperature of the growth environment on diamond habit. *Diamond and Related Materials,* **8** (1999), 1444-1450.

MODELLING AIRBLASTS IN A LONG TUNNEL WITH SURFACE ROUGHNESS

Mining

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Description

- Airblasts due to the collapse of rock are extremely hazardous occurrences and can cause death and damage to mining equipment and infrastructure. The second Mathematics in Industry Study Group in 2005 developed models for the increase of air pressure due to the collapse of rock in an underground excavation. It was found that the rise in pressure is not very large. The next step is to model the flow of air in a tunnel with surface roughness connected to the excavation. If the tunnel is sufficiently long for turbulent dissipation to be significant then a model due to Fanno for turbulent compressible air flow in a tunnel could be applicable. The Study Group was asked to:

  a) investigate if the parameters for typical mining problems lead to the Fanno regime

  b) investigate a Lie group analysis of the full Fanno model and of asymptotic reductions of the mode.

Executive summary

- In the Fanno model for turbulent compressible air flow the mass and energy equations are the same as in the classical inviscid model but the momentum equation has an extra term due to wall drag. The wall drag is an empirical result which can be deduced by averaging turbulent boundary layer models. It damps the flow over large distances but has relatively little local effect. Fanno flow will therefore be applicable if the surface is sufficiently rough for the flow to be turbulent and if the tunnel is long enough for wall drag to be important. The aspect ratio of the tunnel (ratio of diameter to length) must therefore be small. In one industrial application of Fanno flow, to the air-jet spinning of polymer filaments, the aspect ratio was 10^{-3}.

A Lie group analysis of the full Fanno model was not attempted because of the complexity of the problem. However asymptotic reductions of the model have been derived by Ockendon et al (2001). Two equations were identified for Lie group analysis, a nonlinear wave equation which was shown to have three Lie point symmetry generators and a nonlinear diffusion equation. Work on the Lie group analysis and the calculation of group invariant solutions is continuing.

Reference

Ockendon, H, Ockendon,J R and Falle, S A E G. The Fanno model for turbulent compressible flow. *J. Fluid Mech,* **445** (2001), 187-206.