Ill-posed Problems in Product and Process Design

Computational Linear* Algebra for PDEs
The University of Durham,
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P.S. Hope nonlinear problems are admissable!

While I provide Consultancy to Pilkington, and believe some of the examples are important for the future of the wider glass industry and beyond, MY INVOLVEMENT HERE IS PERSONAL

However it does draw from Pilkington experience, with their permission, as well as other sources.

APPLIED MATHEMATICS: Julian Hunt – past president IMA in his Presidential Address:

“Most interesting mathematics now involves Inverse Problems“, or words to that effect

WHY Forward Problems

WHERE Diagnostic Inverse Problems

HOW Inverse Design Problems

Diagnosis: detecting whether something exists, and if so finding the detail

Design: finding if something can be made, and if so how, if not finding an acceptable substitute

May be the same equation

– but a very different philosophy

Concentrate here on Design involving PDEs
- **almost always ill posed in the Hadamard sense**
- **often not amenable to standard regularisation**
- **rarely suited to parametric optimisation**
- **relevant to both products and processes**

This is Industrial Mathematics – with the emphasis on the PROBLEM not the mathematics

I take in my historical order – mostly also the order in which they became worth doing
The first is in fact Diagnostic and Meteorological, but makes a good starting point

1962 – Finding Geostrophic Flows

Then Design and Industrial

1966 - Turbine Blade Design
1970 - Electrochemical Machining
1974 - Mold Design
1978 - Heating Aircraft Screens
1982 - Canal Cooling Control (DPCS)

....

2000 - Making Car Windscreens
2004 - Making Non-circular Tubes

1962 – Finding Geostrophic Flows

Weather forecasting is easy
– if you know what the weather is now

In those days of a 2 layer model
one updated the estimated mid-height transverse pressure distribution using 'radio-sonde' data and found the corresponding streamline flow

$$\mathrm{div}(f\ \mathrm{grad}\ \psi) + 2(\psi_{xx}\psi_{yy} - \psi_{xy}^2) = \mathrm{div}(g\ \mathrm{grad}\ h)$$

(f is the earth's local rotation)

Ellipticity requires:

$$f^2/2 + f\ \mathrm{div}(\mathrm{grad}\ \psi) + 2(\psi_{xx}\psi_{yy} - \psi_{xy}^2) > 0$$

Outside the Tropics (not included at that date)

$f \text{ grad } \psi) = g \text{ grad } h$

provides a good enough estimate to adjust

div(g grad h) **by modifying** h

However weather forecasts are sensitive to any internal inconsistences in the data and it must be done with caution

An opposing compromise is that the numerical results get rougher as the equation becomes closer to becoming hyperbolic

The equation is sufficiently non-linear to require a full convergence analysis of the linearisation used – not repeated here – to develop a reliable algorithm

THE OUTCOME

1. The numerical solution must be absolutely robust to incorporate within each step of a numerical weather forecast, while taking as few liberties as possible in adjusting the data to avoid superficially hyperbolic regions.
2. At that date numerical methods themselves were in their early days – this may have been one of the earliest applications of ’A D I’ methods
3. Nevertheless the discretisation and solution algorithm proved robust in every respect

1966 - Turbine Blade Design

At this date the preferred shape profiles at low Mach number were still hard to determine, and the design target was presentied in terms of the surface velocity

In terms of a stream function ψ this satisfies Laplaces equation in an infinite region with ψ and $d\psi/dn$ **specified at the boundary BUT this is undetermined and to be found**

As a free boundary problem this is not necessarily as ill posed as other problems considered here

It is instructive to note that:

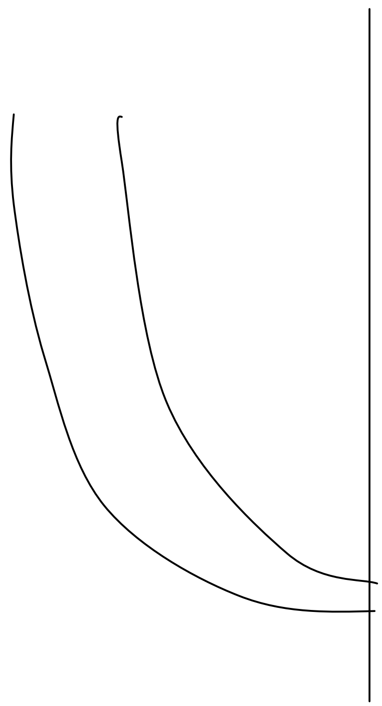
A generalisation of the Joukowsky aerofoil to singularities along the centre line was satisfactory for thin blades

For thicker blades singularities on the boundary positioned opposite with respect to the centre line proved satisfactory

Near analytic methods for design are limited to water & low Mach no. gas/steam turbines

Interest moved to 'streamline curvature' with a less direct approach to the inverse problem

1970 - Electrochemical Machining
1974 - Mold Design



The same axisymmetric problem

To produce a hole to the outside profile,
find the inner tool profile so that
with electrolyte between, the advancing tool gives the desired shape OR

To press a TV tube neck to the inner profile, find the outer water cooled mold boundary so that at the inner boundary the necessary temperature T **(to ensure good surface quality) AND heat transfer to match that from the glass are obtained**
v **(or** T) **satisfies Laplaces Equation**
On the outer/inner boundary v **(or** T**)**
AND dv/dn **(or** dT/dn) **are specified**

v **(or** T) **is specified on the boundary to be found**

Laplaces Equation is to be integrated given ’initial conditons’ and the problem is ill-posed

Hewson Browne at Sheffield in particular drew on astrophysics experience to produce analytical solutions to the machining problem.

Fortunately the practical problems are near to 1D perpendicular to the defined surface, giving:
An initial estimate of the undetermined boundary
A predictor-corrector algorithm adequate for the design pupose and used for the press tooling

Further work on ECM was at the then PERA and I do not know how important this treatment was in their subsequent developments

1978 - Heating Aircraft Screens

**The mathematics dates from 1968,
but the process was still an idea,
and 'took off' in around 1978**

One puts down a coating with an appropriate distribution of conductivity σ

**Busbars at top and bottom supply current with controlled voltages, say V & 0 (zero)
Aircraft screens are bent but near enough developable surfaces to use flat co-ordinates**

THE PROBLEM

A sputtering process was used to provide a conducting coating

This involved setting up an array of cathodes to achieve the required distribution of σ

A handful of people developed the skill and experience to put down a uniform grading

BUT the Trident, 747 and suchlike clearly required a 2D distribution

They could not find a good enough set-up to achieve the requirement of uniformity of heating to around +/-5%

$\mathrm{div}(\sigma\ \mathrm{grad}\ v) = 0$

Uniform heating H **is required**

$(\sigma\ \mathrm{grad}\ v\ .\ \mathrm{grad}\ v) = H$

σ can be found after solving

$\mathrm{div}(1/(\mathrm{grad}\ v.\ \mathrm{grad}\ v)\ \mathrm{grad}\ v) = 0$

Unfortunately this is hyperbolic – other problems involving $(1/\mathrm{grad}\ v.\ \mathrm{grad}\ v)^m$ **are mostly in the elliptic range** $m<1/2$

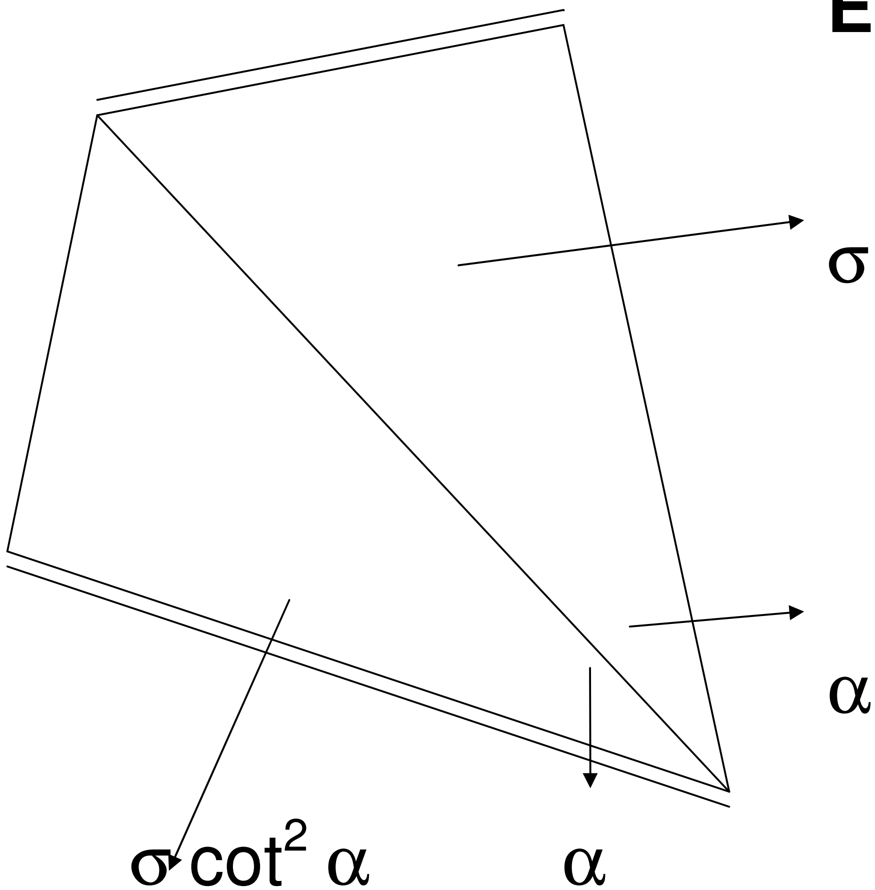
The equation applies also to power law fluids, exceptionally in the hyperbolic range

It is closely related to the compressible flow equation.

The approach I used was newish at the time and published for compressible flow in the Intnl. Jnl. of Num. Meth. in Eng. The ill posed problem was too way out for the SIAM Journal

This idea will re-appear and is now almost the norm so some detail is given in this case.

HOWEVER there are ?surprisingly? some EXACT SOLUTIONS



The basic unit can be built up into a variety of exact solutions

It illustrates the need for a discontinuity in σ at anything but a right angled corner

It is 'easy' to achieve uniform rather than zero heating in an acute angled corner and to avoid a singularity in heating at an obtuse angled corner

This understanding is useful in itself – but not enough
HOWEVER a non-trivial test case is useful

The iterations which are natural for the elliptic problem extend to the hyperbolic one surprisingly well

$$\mathrm{div}(\sigma_n \,\mathrm{grad}\, v_n) = 0$$

Uniform heating H **is required**

$$\sigma_{n+1} = H \,/\, (\mathrm{grad}\, v_n \,.\, \mathrm{grad}\, v_n)$$

We assume a solution σ **exists and throughout the iteration we can linearise using** $\sigma + \varepsilon$

We seek eigenfunctions for ε satisfying

$\varepsilon_{n+1} = \lambda \varepsilon_n$

and with no great difficulty find is λ real

For -ve m $2 m </= \lambda <= 0$

For +ve m $0 </= \lambda </= 2 m$

The iteration converges for $|m| < ½$

The elliptic case with $m < -½$ **requires**

$\sigma_n + \alpha (\sigma_{n+1} - \sigma_n)$ **with** $\alpha < 1$

The hyperbolic case $m>1/2$ **gives**

$0 </= \lambda </= 2 m > 1$ **and** $0 </= \lambda </= 2$ **for** $m=1$

However we can still achieve convergence!

The above iteration implicitly assumes
grad v_n **is a useful approximation**
Consider elongated regions with substantially 1D along the length
The assumption is good for long closely spaced busbars
For short widely spaced busbars the current σ_n grad v_n **should give a better approximation than the voltage gradient**
An alternative iteration would be

$$\sigma_{n+1} = \sigma_n^2 \text{ (grad } v_n \text{ . grad } v_n) / H$$

The eigenfunctions ε_n **are unchanged BUT with the eigenvalue** λ_n **changed to** $2 - \lambda_n$

Using $\sigma_{n+1} = H / (\text{grad } v_n \,.\, \text{grad } v_n)$

And then $\sigma_{n+2} = \sigma_{n+1}^{\;2} (\text{grad } v_{n+1} \,.\, \text{grad } v_{n+1}) / H$

Gives eigenvalues $\lambda_n(2 - \lambda_n)$

Since $0 </= \lambda_n </= 2$ **,** $0 </= \lambda_n(2 - \lambda_n) </= 1$

This is a non-divergent iteration and λ_n **close to** 1 **correspond to** ε_n **with near uniform** H

Using a standard finite volume discretisation the iteration runs as expected, giving more uniform H **at the cost of increasingly rough** σ

One can accelerate the iteration and smooth v **BUT a few iterations of the above gave enough guidance for a skilled operator to set up for a new screen with no great difficulty**

THE OUTCOME

1. A few iterations of the above on a coarse mesh proved sufficient guidance for a skilled operator to set up the process for a new screen without difficulty

2. As the individual cathode opertation became more reliable, I wondered about developing the code to specify the set-up directly

3. The feeling was that cathode behaviour was understood empirically but difficult to model

4. With very little change, the code was crucial in developing new screens for over 20 years – I think now alternative technologies are used.

1982 - Canal Cooling Control (DPCS)

It is necessary in making – for example – bottles to have a very uniform temperature

This may be 200-300C below the temperature at which the glass can be taken from the furnace

The glass is carried along a canal of more or less rectangular cross section with a free surface in slow viscous flow: it can only be cooled (and if necessary re-heated) at the top and side boundaries

What is the shortest length of canal necessary? A constraint is that the boundaries must be kept above the 'devitrification' temperature at which crystals start to form

This type of 'Distributed Parameter Control System' was being widely explored at the time

The straightforward answer is
Cool initially to an average below the target
Reheat the boundaries with a small overshoot
etc. giving optimum operation with alternating cooling/heating steps of reducing length

The practical plant designer finds this impractical - and of little potential benefit
The standard approach is in summary to cool as fast as possible to the required average: then avoid further boundary heat transfer

A related problem I was not aware of then is: Towing a long line with for example sounding equipment, bring it back to straight in the shortest possible distance after a turn
I suspect (but do not know) that a skipper will instinctively run with the optimum overshoot and series of ever shorter correcting moves

2000 - Making Car Windscreens

The bending process is old
The mathematics dates from 1990 as the required shapes became more complicated

One sags the glass at around 600C supported round the edge, controlling temperature and hence viscosity μ over the area so it sags to the target shape

Car windscreens now have too much cross curvature to treat as developable surfaces

There is an alternative process
A key decision is whether sag bending can or cannot make a new product
Getting this wrong can be VERY expensive

The ’forward’ problem is non-linear and the inverse design problem for μ is normally of mixed type

The problem considered explicitly here is the elastic bending of a flat rectangular simply supported plate to a specified small deflection

This 4^{th} order linear inverse problem, unlike the earlier 2^{nd} order non-linear one, was published in SIAM

Philipp Kugler, SIAM J. Appl. Math. Vol.64 No.3 pp858-877

This was a result of an outstandingly successful outcome of EEC funding through ECMI for academic interchanges, in this case between Linz and Oxford

The governing equation - to be regarded as an equation for E, not w is

$$[E(w_{xx}+\nu\, w_{yy})]_{xx}+[E(w_{yy}+\nu\, w_{xx})]_{yy}+2(1-\nu)(Ew_{xy})_{xy} = f$$

The visco-elastic analogy:

For small displacement problems in slow viscous flow the velocity v **can often be found as the displacement** w **in the geometrically identical problem elastic problem taking:**

$E = 3\mu$, $\nu = ½$

Looking ahead, the sag occurs on a support which matches the edge of the windscreen and is NOT flat

The elastic problem remains well defined despite the developing contact - the viscous time dependent problem does not

The above is one reason for working with the elastic inverse problem, despite the possible need for some iterative refinement.

Another attractive concept is that the bending might be thought of as a 2 stage process:

1. **Bending to a developable surface on the support**
2. **Cross curvature developing only within what can be regarded as a linear perturbation on this surface – an approach found to be of great value considering the simpler 1D problem for the vertical centre line**

Philipp worked on the same philosophy as used for the heated windscreen: assume a solution exists and seek a convergent iteration

A demonstrably reliable iteration comes most easily (after reformulating the equation with $\nu = \tfrac{1}{2}$ **) as:**

$$[E(w_{xx}+ w_{yy})]_{xx}+[E(w_{yy}+ w_{xx})]_{yy} +[Ew_{xy}]_{xy} - (Ew_{yy})_{xx}/2 - (Ew_{yy})_{xy}/2 = f$$

$$E_{(k+1)} / E_{(k)} = 2 -[w_{(k)xx}\, \mathbf{w}_{xx} + w_{(k)yy}\, \mathbf{w}_{yy} + w_{xy}\, w_{xy} + w_{yy}\, w_{xx} /2 + w_{xx}\, w_{yy} /2] / [w_{(k)\,xx}\, \mathbf{w}_{xx} + w_{(k)\,yy}\, \mathbf{w}_{yy} + w_{xy}\, w_{xy} + w_{yy}\, w_{xx} /2 + w_{xx}\, w_{yy} /2]$$

Having seen this, but noting it does not reduce to the non-iterative exact solution in the 1D case, my inclination is to develop this giving:

$$E_{(k+1)} / E_{(k)} = [w_{(k)xx}\, w_{xx} + w_{(k)yy}\, w_{yy} + w_{(k)xy}\, w_{xy} + w_{(k)yy}\, w_{xx} /2 + w_{(k)xx} w_{yy} /2] / [w_{xx}\, w_{xx} + w_{yy}\, w_{yy} + w_{xy}\, w_{xy} + w_{yy}\, w_{xx} /2 + w_{xx} w_{yy} /2]$$

The former uses solely the latest Total Curvature: the latter seems more likely to be robust in the regions where this is small and the Cross Curvature is the more significant

THE OUTCOME

An attempt at standard regularistion failed due to the numerical problems of consistent evaluation of high derivatives in the FE code

Some guidelines have been found

However I believe normal practice is using parametric methods which may work well BUT can be very unsatisfactory

At least trial and error is a lot cheaper on a computer than on production plant!

Philipp's paper and examples suggest a hopeful line of approach – but it has yet to be shown it is robust for products of interest

2004 - Making Non-circular Tubes

Glass tubes such as those used for fluorescenrt lighting are circular

They are drawn from an annular orifice
OR from a rotating mandrel

They are carried for many metres on rollers before they are cool enough to cut
Back-pressure from an internal gas flow along them and a slow rotation about the axis as they travel keeps them circular

For a period of some years modelling workshops were run by the Glass SIG of ECMI Schott raised the problem of forming other sections - for example square tubes

The internal pressure and additionally surface tension (ST) tend to keep a tube round: rotation avoids gravitational flattening

Other shapes clearly need minimal or negative excess pressure. That tends to be unstable but 'upstream' integration of the equation for profile development is possible

HOWEVER incorporating ST the integration is grossly unstable – over short wavelengths falttening is very fast – and unstable growth of roughness integrating upstream.

Various participating groups looked at this with some resulting publications. I think a fair summary is that rather than regularising the problem it is better to:
Integrate the equation upstream with zero ST to give a suggested feed shape,
then downstream including ST

The upstream intgration with zero ST then provides the basis for a predictor-corrector algorithm

This applies to the process using an orifice which can define the initial profile

THE END

With thanks for your interest in this type of industrial application of some of the problems being studied in this Durham Symposium

SUMMARY

1. Ad hoc iterative methods can work surprisingly well for ill posed design problems

2. However the iteration must be carefully chosen with appropriate convergence parameters

3. As for the NS equations (unless the interest is in instability phenomen as in meteorology), discretisations should tend to err towards being ’more elliptic’ / ’smoother’ than the equation