Vector Fields European User Group
Oxford 2002

"Application of Opera to modelling NMR magnet systems"

Peter Aptaker
Laplacian Limited
Abingdon

or

The *open*Garfield Magnet

Or

"Watching paint dry"

(Prize for first to guess why?)

1 Laplacian Limited

1.1 Company Background	*1.2 Business Areas*
Laplacian was formed to exploit the founders 28 years in magnet technology especially 17 at the forefront of modelling and design in NMR systems.	• High technology magnet designs, consultancy and small scale production • NMR systems especially gradients, shims and magnets • Niche magnets (e.g. Garfield magnet) • Specialist data processing and analysis (e.g. NMR related Inverse Problems) • Analytical solutions • Vector Fields parameterisation, interfacing (e.g. Excel) and optimisation

2 This talk

Brief overview of 18 months (?) applying Modeller to NMR magnet systems

- Mainly on the openGarfield magnet
- ***Brief*** overview of Modeller for NMR

… there will be no time for

- Leo: Laplacian Excel Opera interface (4-post magnet example)

3 Strafi Background

Strafi **(Stray**–field) Imaging performing NMR experiments in the fringe field beyond the end of (homogenous) super-conducting magnets where there is both a high gradient and significant field.

It is useful for specialist thin film NMR e.g.

- In use effectiveness of solvent-borne coatings
- Curing (e.g. wood)
- Applications can monitor diffusion and profile T1 and T2 with over depth and time

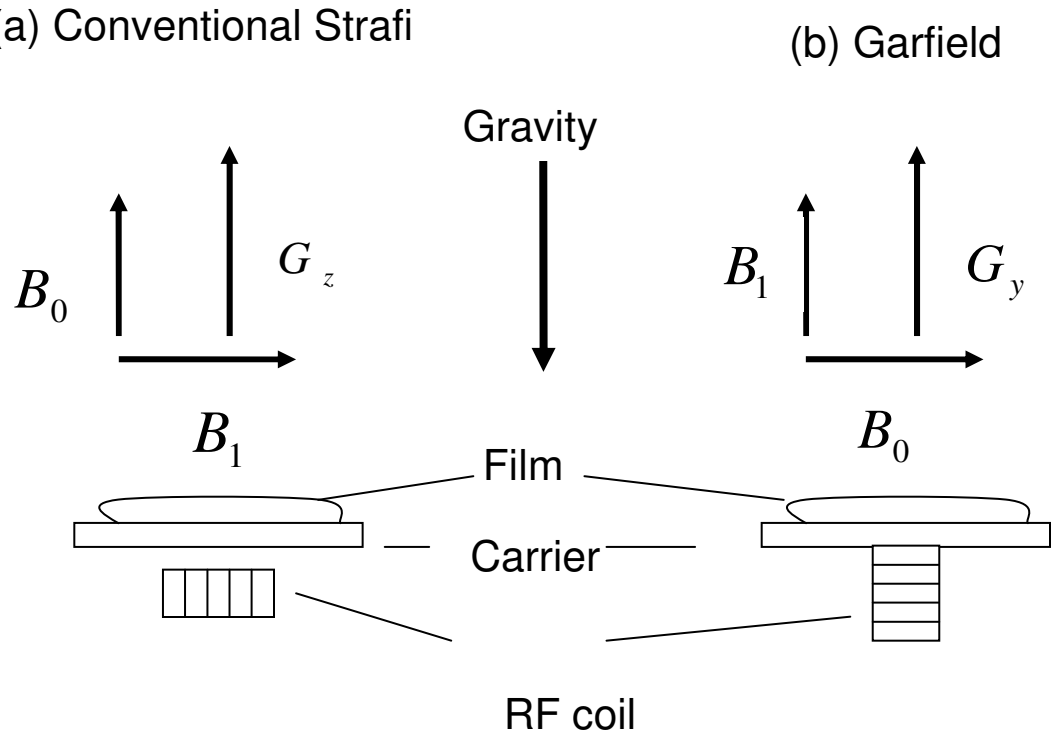
4 Garfield background

(Prize if you can guess the acronym!?)

1997	Conceived by Paul Glover and Peter McDonald (at University of Surrey): Garfield is a permanent magnet designed to offer all the features of Strafi (and more) and lower cost.
1997	First Garfield designed by P.S. Aptaker at Resonance Instruments
1999	see “A Novel high-gradient permanent magnet for the profiling of planar films and coatings”, P.M. Glover, P.S.Aptaker, J.R. Bowler, E. Ciampi and P.J. McDonald”, J. Mag. Res, 139, 90-97 (1999)
2002	Latest openGarfield designed by P.S. Aptaker at Laplacian

5 Strafi and Garfield Configuration

Two possible geometrical configurations of relative directions of static field (B_0), gradient (G) and RF field (B_1). Note B_0 and B_1 are always orthogonal.



6 Garfield Original Specification

- A simple permanent magnet system (no running costs, plugs into standard bench-top spectrometer)
- “large” useable volume and access
- A horizontal field of typically .8T (c 30MHz)
- A deliberate gradient (e.g. 20 T/m)
- As uniform |B| in plane as possible (This will produce an profile/ image which is not spatially distorted, essential for imaging thin films)

7 The Garfield Solution

Uniform |B| in plane ?

- This is natural solution to Laplace's equation in Cartesian coordinates
- The pole profile should follow from the lines of constant equipotential

8 Pole equipotential equations 1

The Cartesian solution of Laplace's equations gives a scalar potential

$$\phi(z, y) = a \sin(bz) \exp(-by)$$

and magnetic fields

$$B_z = \frac{\partial \phi}{\partial z} = ab \cos(bz) \exp(-by)$$

$$B_y = \frac{\partial \phi}{\partial y} = -ab \cos(bz) \exp(-by)$$

9 Pole equipotential equations 2

The field modulus becomes a function only of height y

$$|B| = a\,b\exp(-b\,y)$$

thus producing non-spatially distorted images despite the extreme curvature of the field.

The wave-factor b defines the gradient to field ratio

$$\frac{G}{|B|} = -b$$

With w is the chosen operating clearance gap, the pole profile is on a chosen equipotential

$$z(y) = \pm\frac{\sin^{-1}(\sin(bw/2)\exp(by))}{b}$$

10 Special resolution error

With the field modulus

$$|B| = a\,b\exp(-b\,y)$$

the derivative is simply

$$\frac{d|B|}{dy} = -b|B|$$

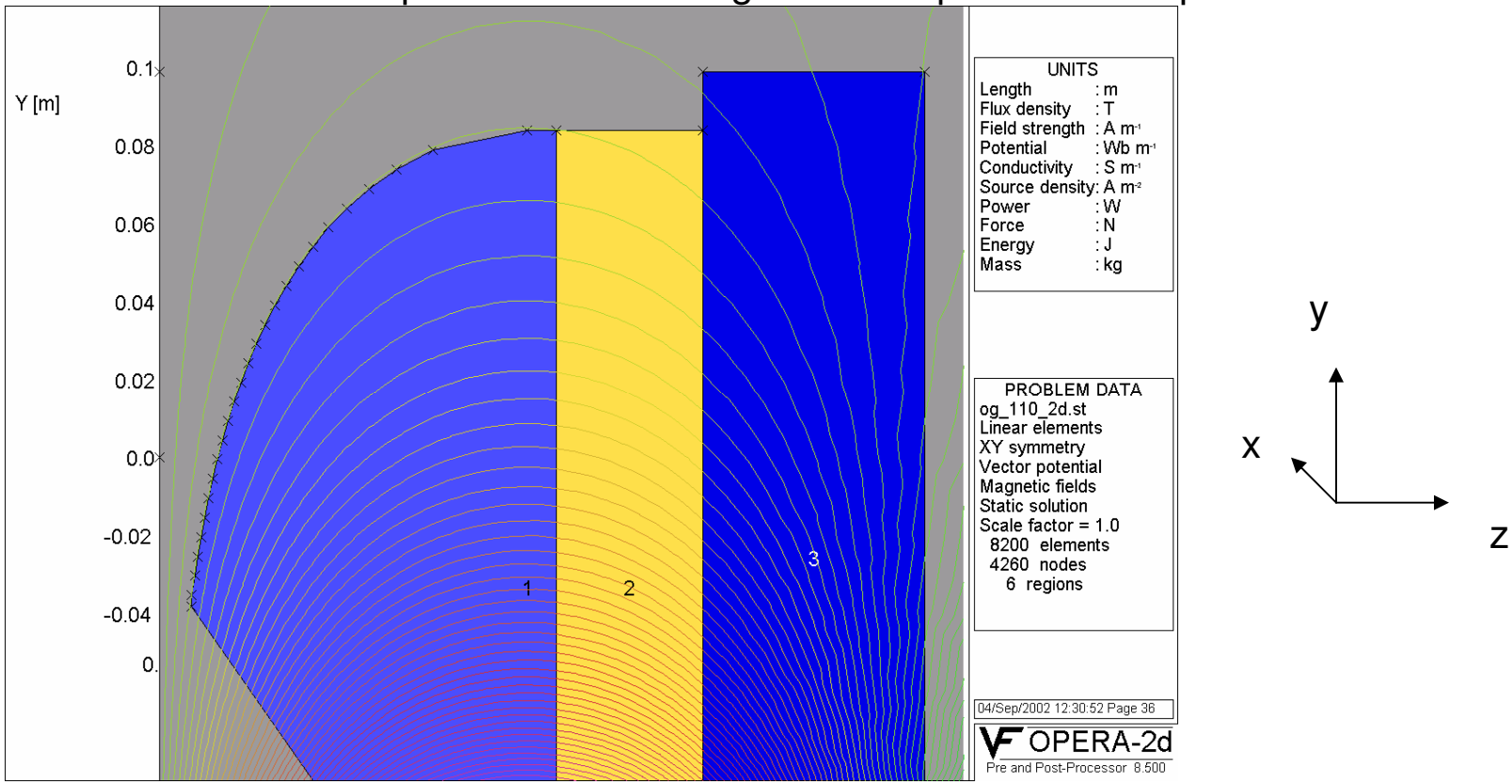
If there is a field error ΔB this will correspond to a special resolution error of

$$\Delta y = \frac{\Delta B}{b|B|}$$

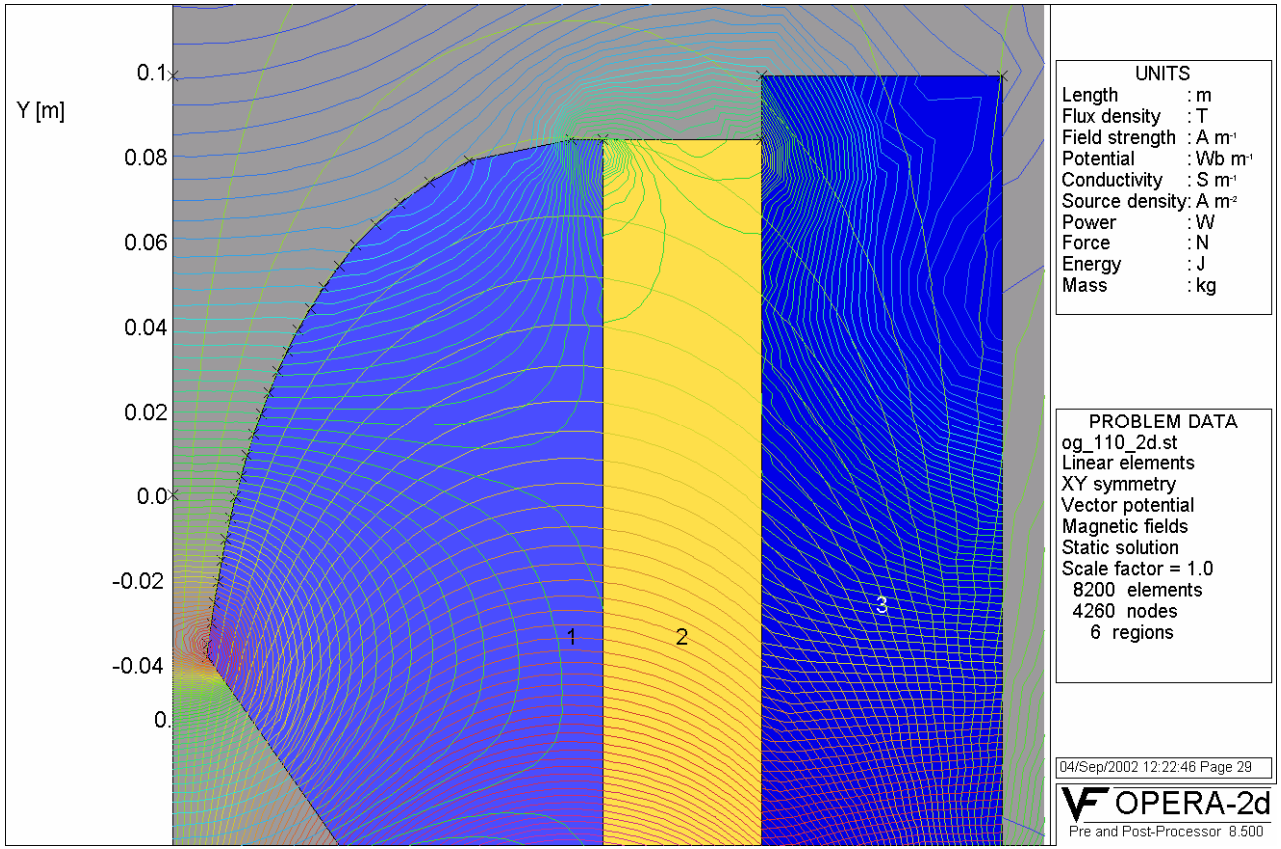
E.g. $b = G/|B| = 17\,m^{-1}$ gives 1/b=.06 m

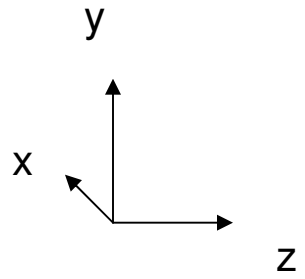
11 Equipotentials of $\phi(z, y) = a\sin(bz)\exp(-by)$

Note: This is NOT the potential of the magnetostatic problem on Opera2D.

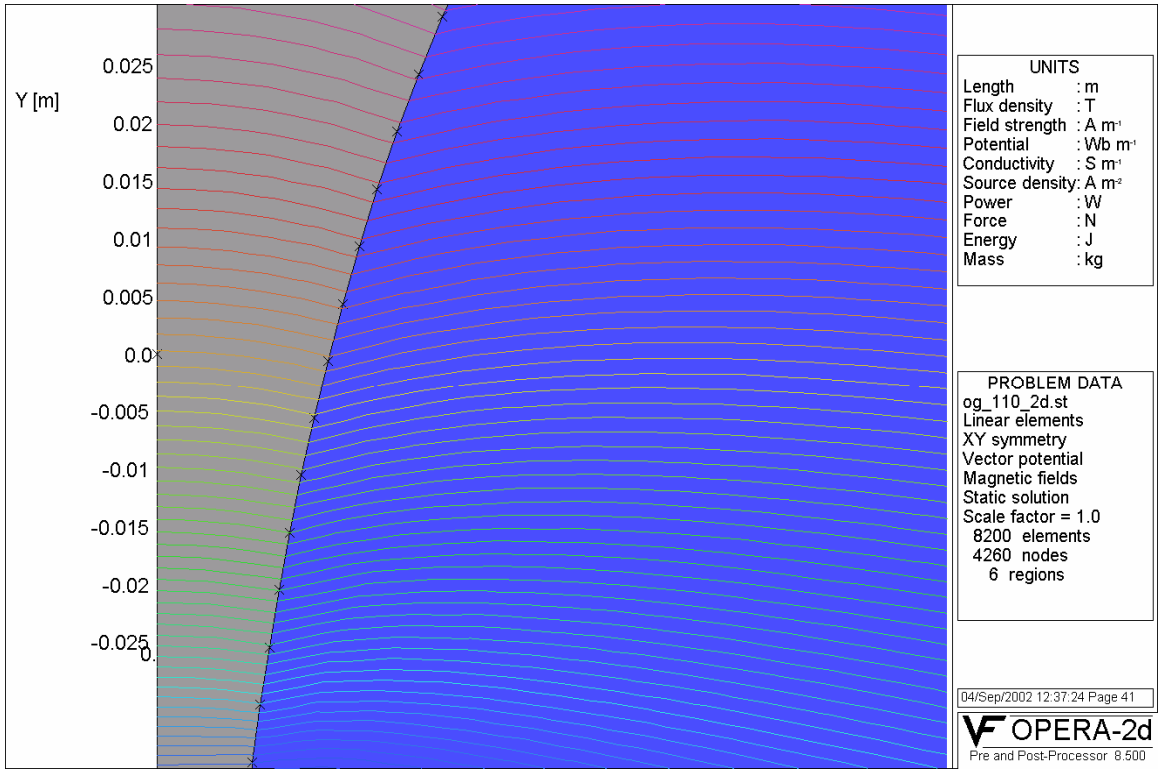


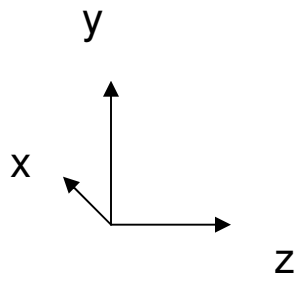
12 Equipotential of $\phi(z, y) = a\sin(bz)\exp(-by)$ and $|B|$





13 The curvature of flux (Vector potential)



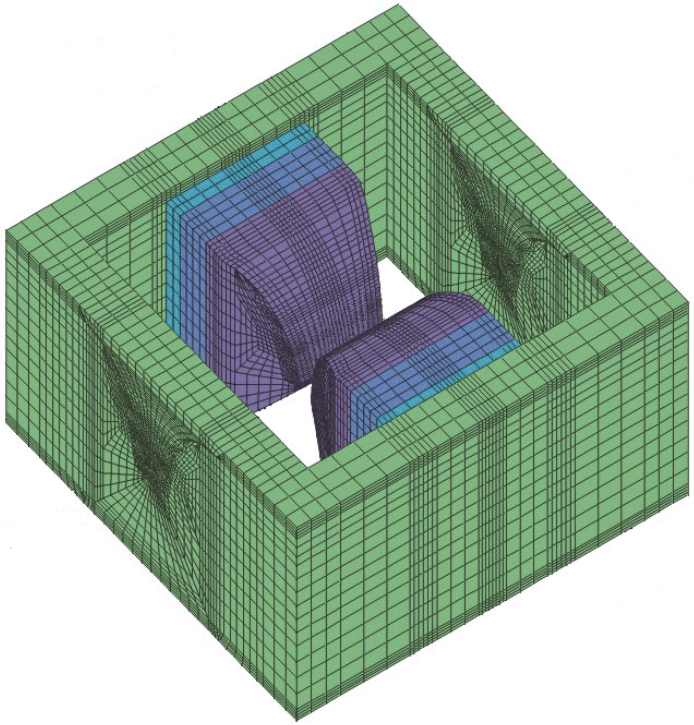


14 Original Garfield Magnet

Summary

- Working field >30 MHz (0.7T)
- G/|B| = 20 T/m
- Clearance >20 mm
- Magnet circuit = closed

Opera model (Pre-processor)



15 Original Garfield Conclusions

Design

- Modelled successfully in Opera2D (paramerised command file)
- Modelled successfully in Tosca (utilising JS written command files)

Implementation

- Built and tested successfully (1998?)
- Within customer resolution specified resolution of 50 μm
- In almost constant use at University of Surrey since then

16 OpenGarfield

Main changes requested included:

- 150% scaling
- Open access (e.g. C-core)

17 Opportunities to outsource and save money?

Buy it

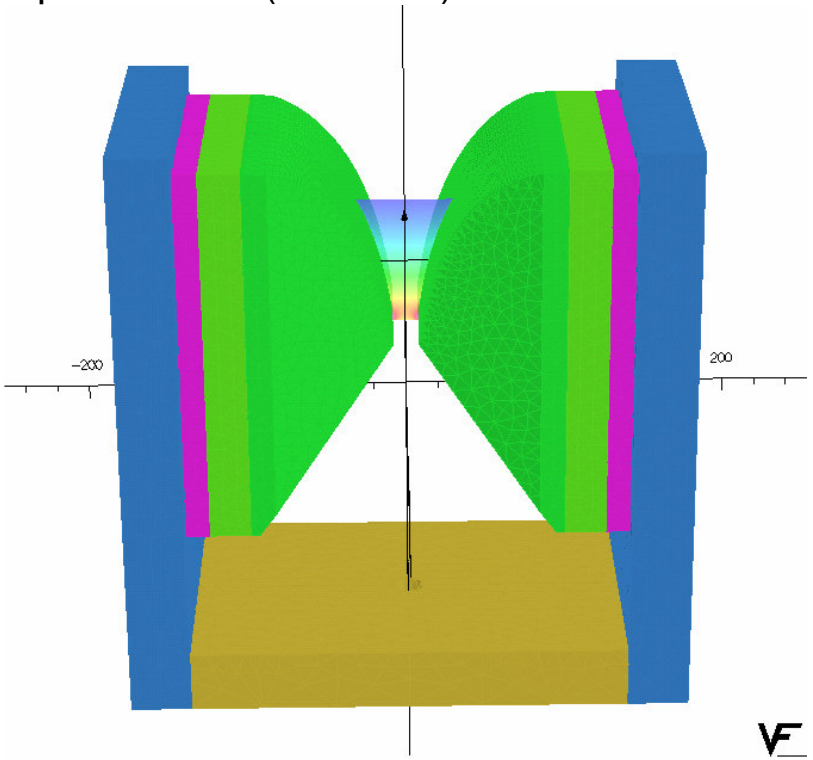
Product Name:	**Garfield Magnet 2**
Our Price:	$3.50
Availability:	In Stock
Product Number:	44022-2
Product Weight:	0.5 lb.
Rating:	★★★★½

18 Open Garfield Magnet

Summary

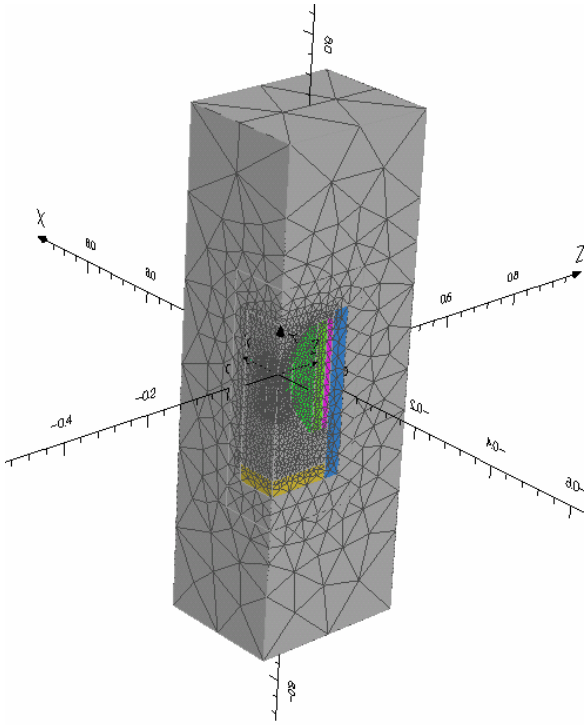
- Designed and supplied by Laplacian Limited
- Working field 30 MHz
- 150% scaling
- G/|B| = 16.6 T/m
- Clearance >30 mm
- Magnet circuit = Open

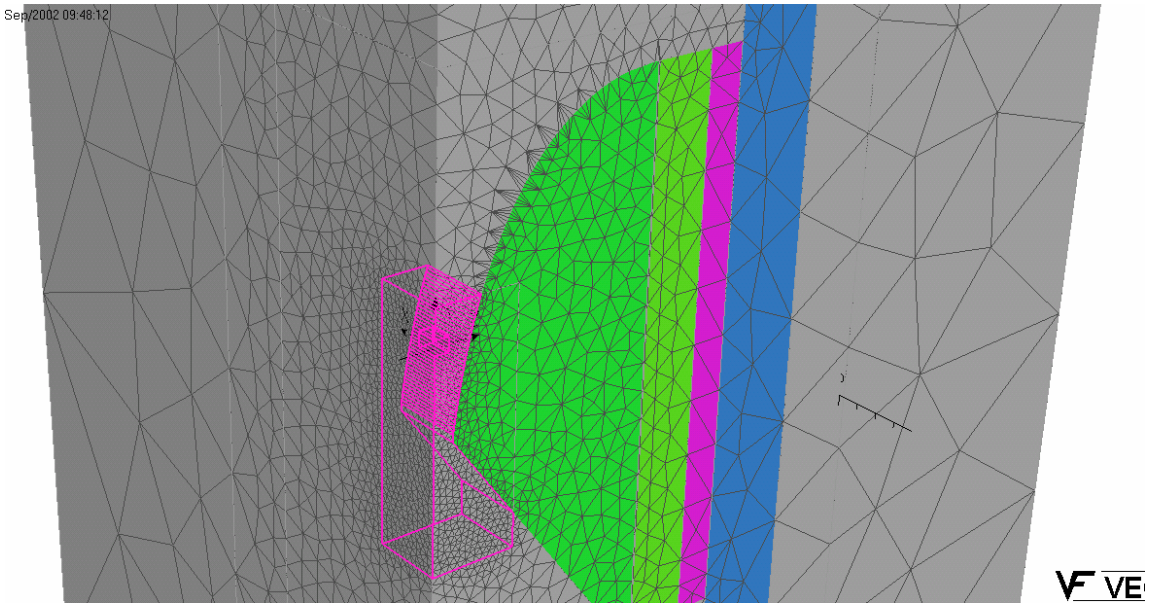
Opera model (Modeller)



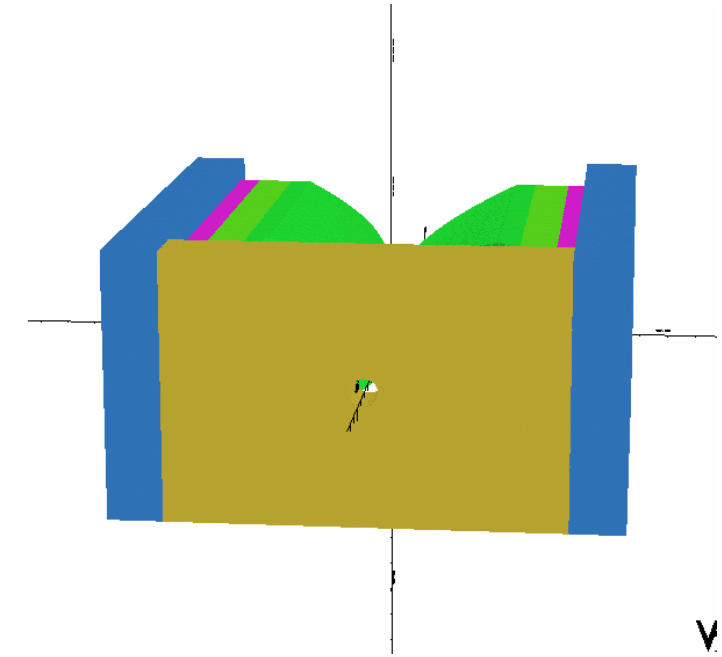
19 Modeller Mesh

Grading with AIR BLOCKS with different LEVELS and mesh length



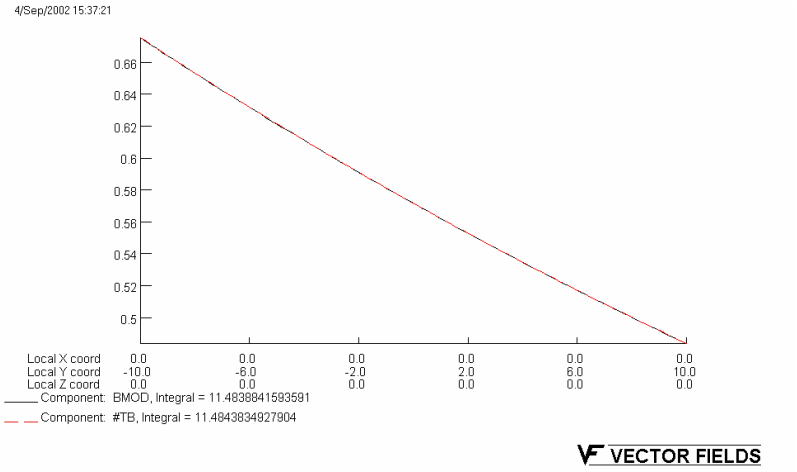


20 An access hole is easily incorporated

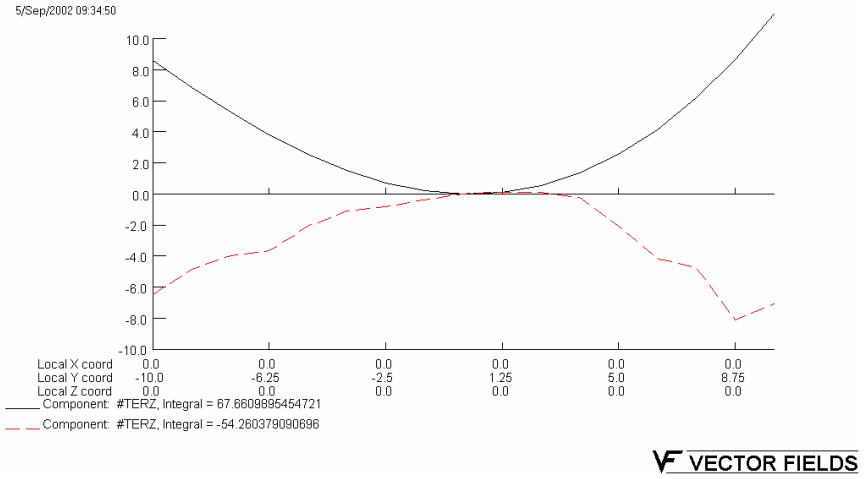


```
.
.
$IF #dhole gt 0
  CYLINDER Name=CUT X0=0 Y0=#y7-10*#mm Z0=0 X1=0
     Y1=#y5+10*#mm Z1=0,MAJORRADIUS=#dhole/2,
     MINORRADIUS=majorradius,TOPRADIUS=majorradius
  PICK ADD NAME SIDE
  PICK ADD NAME CUT
  COMBINE OPERATION=TRIM +REGULAR
  PICK ADD NAME CUT
  DELETE
$END IF
.
.
```

21 Modeller |B| and resolution error as function of height (y): Fields Integral and Nodal (dashed)

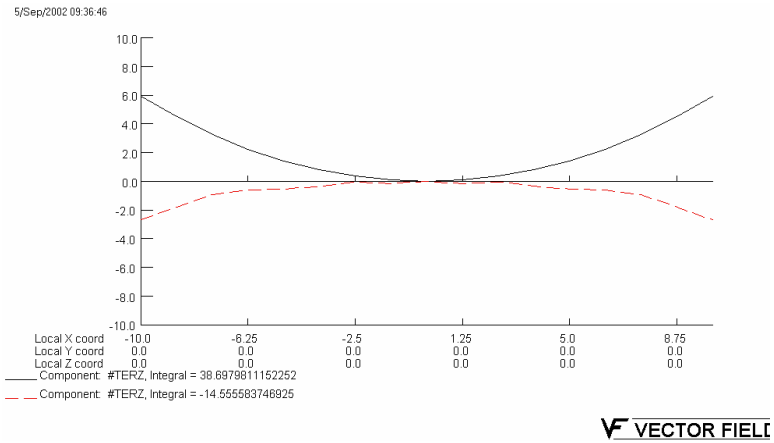


(a) |B| vs. y

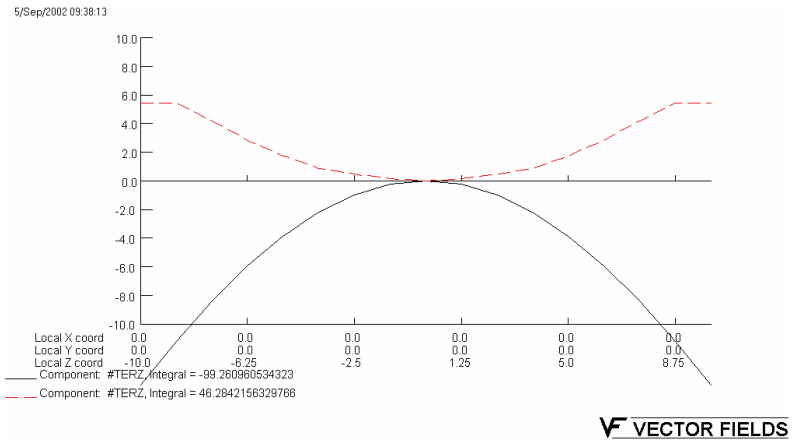


(b) Error (µm) vs. y

22 Modeller resolution error as function of (a) x and (b) z : Fields Integral and Nodal (dashed)



Error (μm) vs. x



Error (μm) vs. z

23 openGarfield magnet: Conclusions

Modeller?

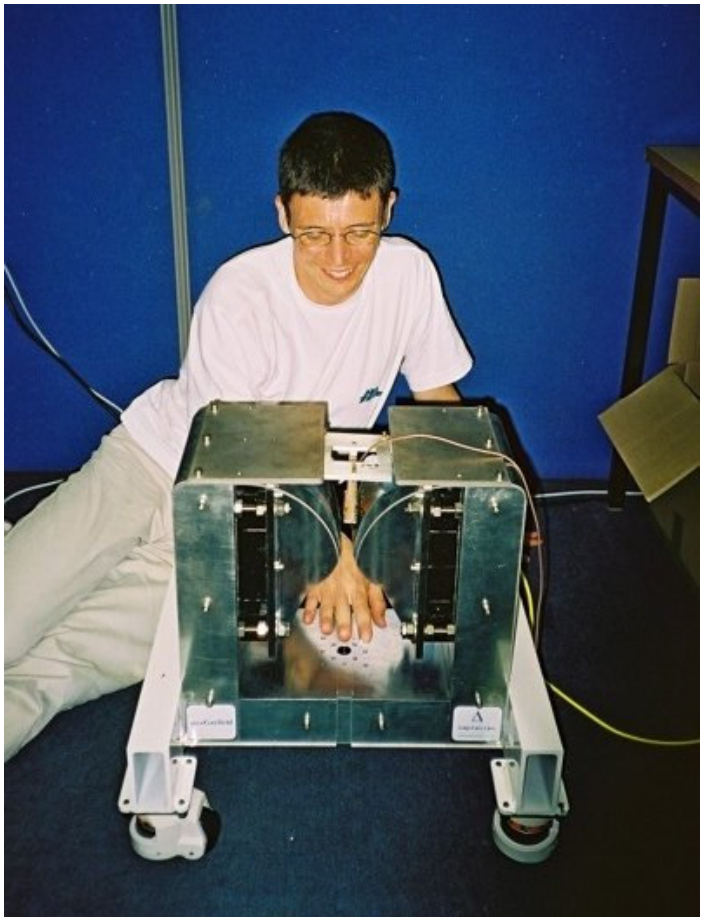
- Modeller facilitated (relatively) easy parameterisation (.COMI files)
- Annoying not (yet) having extrusion (an experienced user may be happier with old pre-processor and hex elements)
- Required Field accuracy was easily maintained (INTEGRAL useful)
- Some meshing problems due to extremes of mesh size

The magnet built successfully e.g.

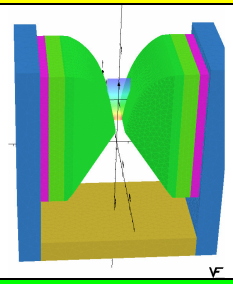
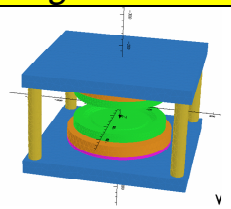
- Assembly forces were not way out (no injuries)
- Fields were as expected
- Customer will begin experiments ASAP

Proud builder!

24 Proud user!



25 Issues with Modeller for NMR magnet systems?

	Garfield	*Bench-top permanent magnets*	*Bench-top NMR probes*	*NMR gradients*	*Shielding*
					
VF 3D code	Tosca	Tosca	Elektra	Elektra	Tosca
Meshing thin regions			****		***
Other Meshing difficulties	*	*		*	
Polygon extrusion need	****	***			
Uniform mesh regions desirable	**	***			
Power in current-carrying conductors?			****	***	
Accuracy Hex vs. Tet?	?	?	?	?	?

26 Accuracy of Opera

User perception?

	Program	***Comment***
	Opera2D.	Most accurate if 2D approximation good
	Opera3D Hexahedral elements	Most accurate if 2D approximation bad
	Opera3D tetrahedral elements	Accuracy challenged?

- Is this view of accuracy correct?
- With improvements in computing power will this perception change?

27 A long decade?

VF European User Meeting	*PSA (almost) annual "lecture"*
1991? (Southampton):	Begged for improvements to 3D pre-processor to facilitate parameterisation and optimisations
1998 (Oxford):	Presented Rio the Opera Interface: complained more about 3D pre-processor ..
1999 (Eindhoven)	PSA almost kept quiet
2000 (Lille):	Modeller beta test offers simple 3D parameterisation
2002(Oxford):	Modeller nearly two years on and Modeller fulfils wildest dreams .. soon

28 Opera wish list 2002

Modeller

- More reliable meshing especially thin regions
- Option for “Uniform” mesh (e.g. Legendre harmonics)
- Integration of tetrahedral and hex elements ?
- Polygon Extrusion

General

- Improved Windows integration (ActiveX and .COM are “old hat”, to be replaced by .NET)

"Watching paint dry"

29 Appendices

30 Skin studies example

With thanks to Paul Glover who supplied these extracts from:

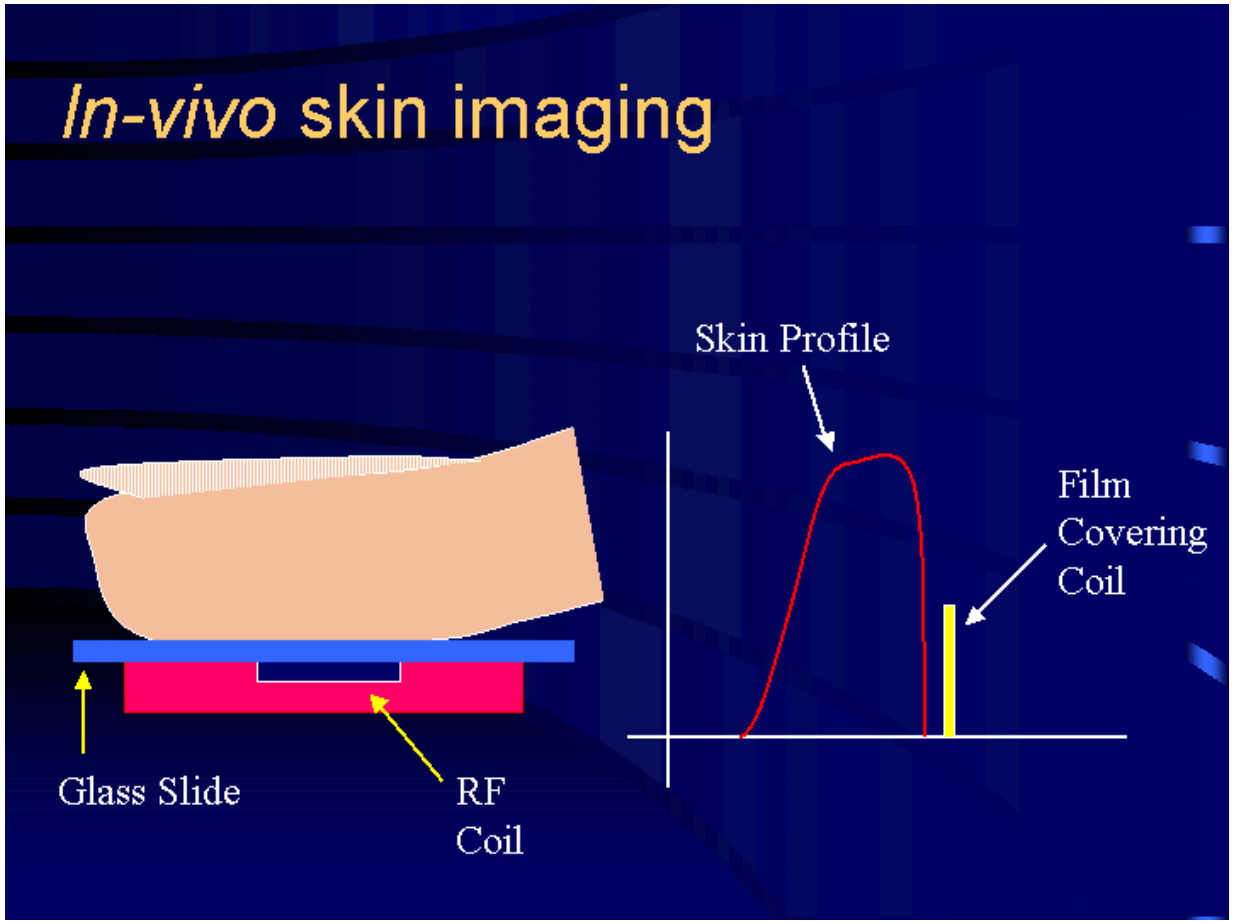
“A high-gradient permanent magnet for Skin Magnetic Resonance Imaging”

P. Glover, M. Dias, J. Hadgraftt and P. McDonald

which discusses:

- Hydration
- States of water and its mobility (free and bound, T1, T2 and diffusion)
- Transport through skin
- Effect of creams (on rehydration or transport)
- Fluorinated (or labelled) drug transport

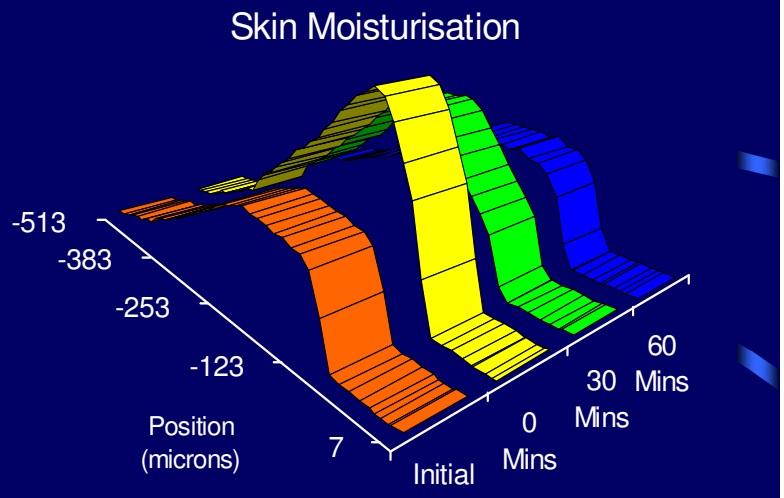
31 Glover et al



32 Glover et al

In-vivo skin studies

- Demonstration of uptake of moisturiser cream and subsequent loss and return to equilibrium



33 Modeller meshing details

Mesh densities

```
 *** COMMENT ********** /mesh length
 *** CONTROL COMMAND ** $CONST     #mlsc   1.0*#lsc
 #MLSC=0.0015
 *** CONTROL COMMAND ** $CONST #ml_air0  #mlsc*0.5
 #ML_AIR0=7.5E-04
 *** CONTROL COMMAND ** $CONST #ml_air1 #mlsc*2
 #ML_AIR1=0.003
 *** CONTROL COMMAND ** $CONST #ml_air2  #mlsc*8
 #ML_AIR2=0.012
 *** CONTROL COMMAND ** $CONST #ml_air3  #mlsc*32
 #ML_AIR3=0.048
 *** CONTROL COMMAND ** $CONST #mlpole   #mlsc*8
 #MLPOLE=0.012
 *** CONTROL COMMAND ** $CONST #mlmag    #mlsc*16
 #MLMAG=0.024
 *** CONTROL COMMAND ** $CONST #mlframe  #mlsc*32
 #MLFRAME=0.048
 *** CONTROL COMMAND ** $CONST #mlbound  #mlsc*128
 #MLBOUND=0.192

Mesh Details

** COMMENT ********** / --------------------------
 *** CONTROL COMMAND ** $if #mesh eq 1
 **** FILE INPUT ******   model create
```

```
 **** FILE INPUT ******   mesh size=#mlbound
 Initial triangulation contained 2569 nodes.
 Volume  facets:     213
 Element facets:   14236
 **** FILE INPUT ******   fill
 TOTAL   volume:0.105446008
 Mesh quality (RMS): 1.035805905  (Worst): 2.05561E-04
 TOTAL vertices:   23981
 TOTAL elements:  135465
 *** CONTROL COMMAND ** $end if
|                                                                              |
 | Job Completed                          :    375.2 s cp,     6.9 m elapsed
```