

Introduction to Multi-physics Modelling

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Computational Modelling of multi-physics processes - What is it?

• Computational Modelling is :

- "The application of numerical approximation methods and computers to the solution of problems in Engineering and Applied Sciences" O. Zienkiewicz
- Computational modelling can be used to predict a number of physical phenomena including:
 - Fluid Flow

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- Heat Transfer
- Solid mechanics
- Electromagnetics
- Etc



Multi-physics involves some or all of the above simultaneously



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Computational Modelling – What is it?

- Simulating real-world phenomena on a computer involves:
 - understanding the governing physics.
 - formulating the problem in terms of mathematics.
 - writing computer software that solves the mathematical equations.
 - running the computer program

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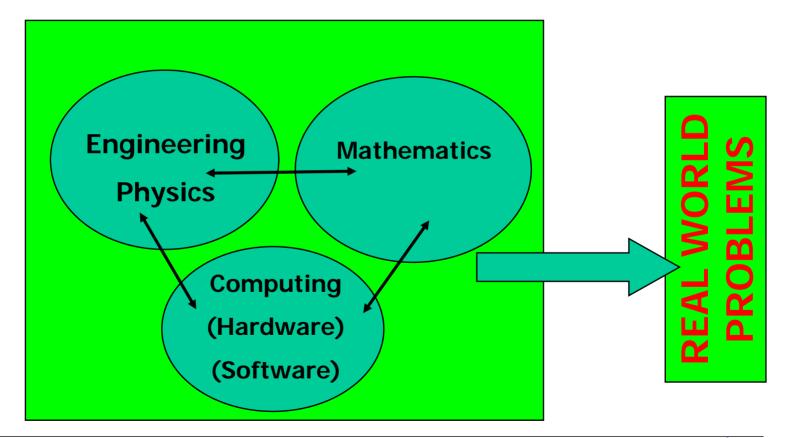
- viewing (& analyzing) the results.
- Generally most real-world problems require solution to thousands of equations.
- Many commercial software tools now available.





Computational Modelling - What is it?

Computational Modelling Research - Interdisciplinary





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Why use Computational Modelling?

\$1,000,000

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Cost of Quality

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- warranty liabilities due to field failures;
- redesign; rework; and scrap costs.

Lateness of product to market

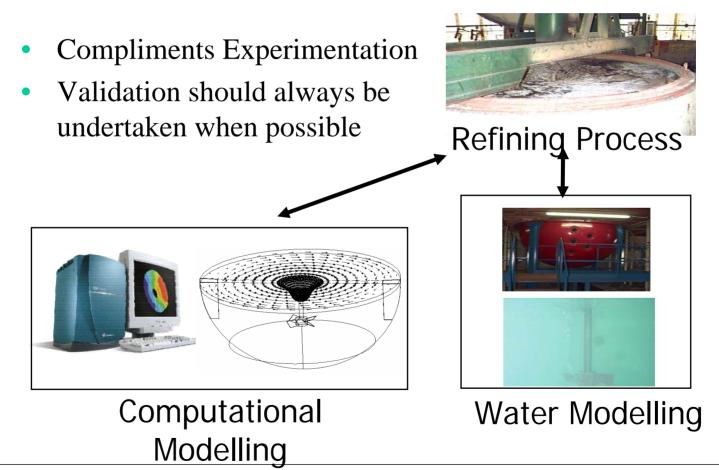
First two manufactures to market lock up 80% of business







Modelling – real world interaction





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Governing Physics

Materials Processing

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- Fluid Flow + Free surface
- Chemical Reactions
- Electromagnetic Fields
- Heat Transfer
- Solidification
- Stress

Many processes governed by interactions of the above

- Multi-physics
- Multi-scale 0.1μ 1m



Refining



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Casting

Governing Equations

• The governing equations can be expressed in a standard form:

$$\frac{\partial}{\partial t} (\rho A \phi) + \nabla Q = \nabla (\Gamma \nabla \phi) + S$$

	ø	А	Γ_{ϕ}	S	Q
Continuity	1	1	0	S _{mass}	$\rho \underline{v}$
Momentum	$\underline{\mathcal{V}}$	1	Γ_{v}	$\left(S + \underline{J} x \underline{B} - \nabla P\right)$	$\rho \underline{v.v}$
Heat transfer	h	1	$\frac{k}{c}$	${S}_h$	$\rho \underline{v} h$
Electromagnetism	<u>B</u>	1	η	$(\underline{B}\nabla)\underline{v}$	<u>u.B</u>
Solid Mechanics	<u>U</u>	$\partial / \partial t$	μ	$\rho_{\underline{f}_b}$	$\mu(\operatorname{grad} \underline{u})^{T} + \lambda(\operatorname{div} \underline{u} - (2\mu + 3\lambda)\alpha T)\underline{I}$



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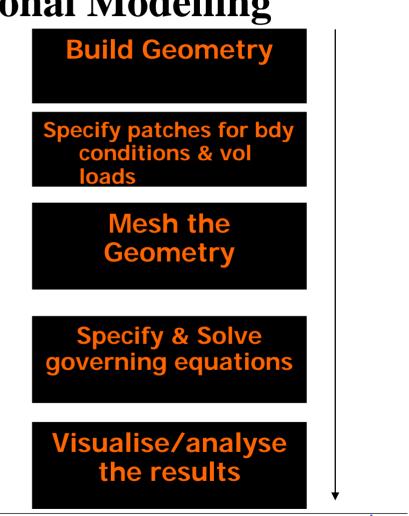


Steps In Computational Modelling

- CAD generates geometry
- CAD captures 'patches'
- CAD domain meshed

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- Number of methods used to discretise equations
 - Finite Difference
 - Finite Element
 - Finite Volume
- Graphically based software tools for results analysis & visualisation.
- 'patches' are points, surfaces or volumes

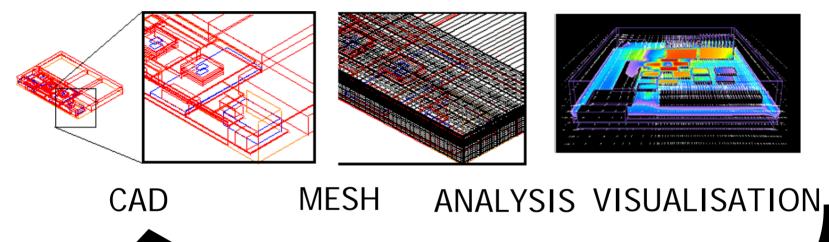






Steps in Computational Simulation

• CAD – MESHING – ANALYSIS - VISUALISATION





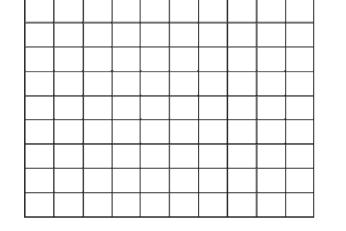


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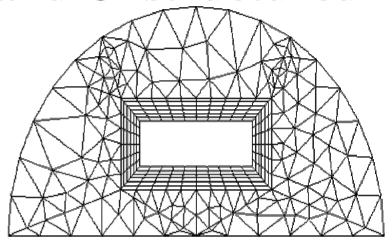




- Data referenced using I,J grid lines
- Allows line-line solvers.

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- Low in-core memory requirement
- Poor on complex shapes.
 - Use BFC or Block-Structured



•Good for complex geometry

- Topology representation
 - Points Faces Elements
- Mix element types.
- Requires whole field solvers.
 - Large memory needed



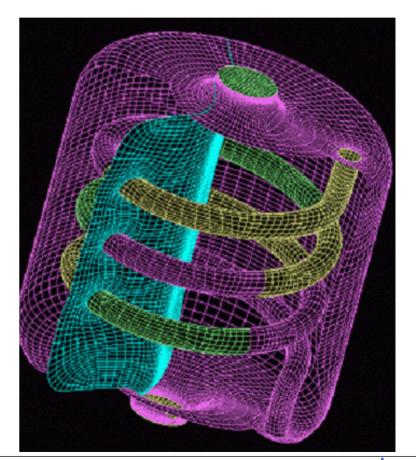




CAD + Meshing Software

• PRO/ENGINEER

- http://www.ptc.com/
- CATIA
 - http://www.catia.com/
- Mentor Graphics
 - http://www.mentor.com/
- FEMSYS
 - http://www.femsys.co.uk/
- GRIDPRO
 - http://www.gridpro.com/





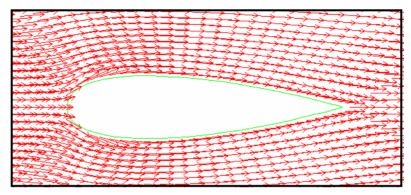


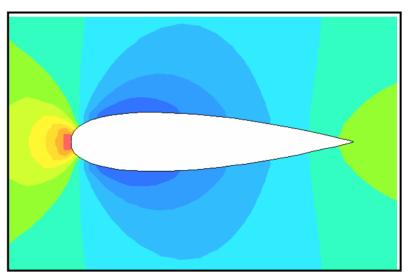
Computational Fluid Dynamics - CFD

- Started in early late 60's early 70's
- Based on Finite Difference/Volume Methods
- Simulations now include
 - Turbulence

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- Free surface Flows
- Heat Transfer + Solidification
- Chemical Reactions
- Early work based on structured grids
- Unstructured Meshes now used
- FE Methods also used.









Computational Fluid Dynamics

$$\frac{\partial \rho \phi}{\partial t} + div(\rho \underline{u}\phi - \Gamma_{\phi} \nabla \phi) = S_{\phi}$$

- **Typically**
- Used Finite Volume Method
- Eulerian Approach (Fluid moves through a static mesh)
- Highly non-linear

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Fluid Flow

$$\frac{\partial \rho u_x}{\partial t} + div(\rho \underline{u} u_x - \mu \nabla u_x) = -\frac{\partial p}{\partial x} + \rho g$$
$$\frac{\partial \rho}{\partial t} + div(\rho \underline{u}) = S_m$$

- Navier-Stokes equation
- Newtonian fluid

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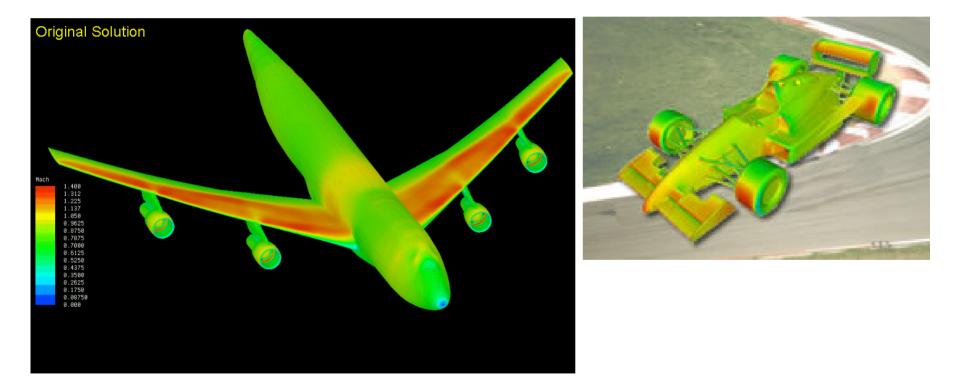
- SIMPLE type algorithm resolve pressure
- Staggered Multi-block Cartesian or cylindrical polars







Fluid Flow





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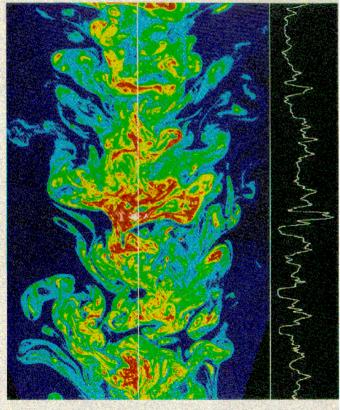
Turbulence

- Solved variables contain a
 - time averaged component
 - fluctuating component
- Turbulence models the effects of the fluctuating component
- Effects other equations by affecting the diffusion coefficient
- Many turbulence models
- k-e most commonly used



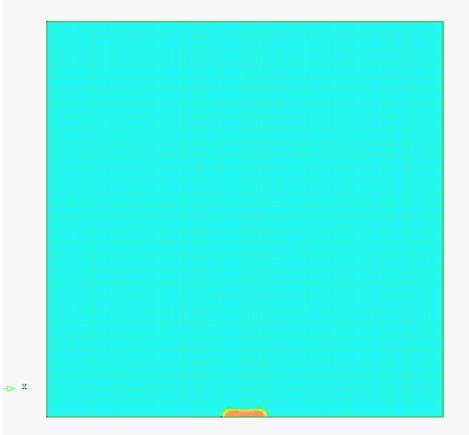






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Figure 23 The result of applying a conformal mapping to the jet shown in Figure 3. The map, due to Everson et al (1990), corrects for the growth of the jet by covering a wedge int a slot. The downstream decay of the mean concentration has been normalized using similarit considerations. The signal to the right corresponds to the vertical line cut shown in the jet.





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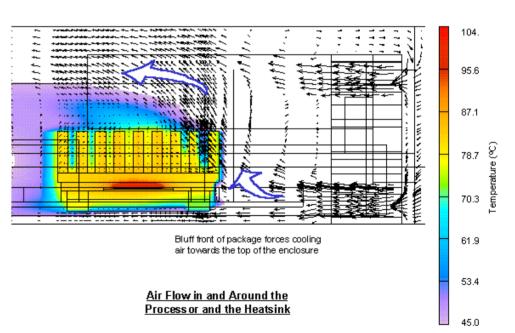


Commercial Software – CFD

- Resources at : http://www.cfd-online.com/
- FLUENT
 - http://www.fluent.com/
- PHOENICS

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- http://www.cham.co.uk/
- STAR-CD
 - http://www.cdadapco.com
- PHYSICA
 - http://www.multi-physics.com
- CFX
 - http://www.annsys.com/cfx





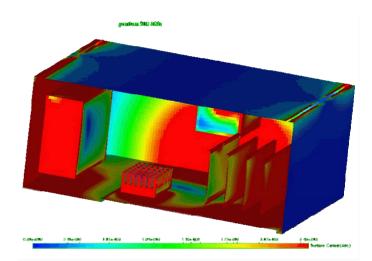


Computational Electromagnetics

- Solution to Maxwells equations
- Low Frequency (10-100KHz)
 - Time dependence importance
- High Frequency (>1MHz)
 - Frequency domain

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- Number of methods used
 - Finite Difference
 - Transmission Line Methods
 - Finite Element Methods



Surface currents at 482MHz





MHD Equations

- Assume I have the NS equations, etc then ADD
- For example a simple derivative form of the Maxwell's Equations

$$\nabla \cdot (\boldsymbol{\sigma} \nabla \boldsymbol{\phi}) = \nabla \cdot (\mathbf{u} \times \mathbf{B}) + S_{\boldsymbol{\phi}}$$

$$\mathbf{E} = -\nabla \phi$$
 and $\mathbf{J} = \sigma_e \mathbf{E}$.

- B from the Biot Savart Law
 - e.g. B = (m I/4p) dI x r / |r|3
- Lorentz force: J x B

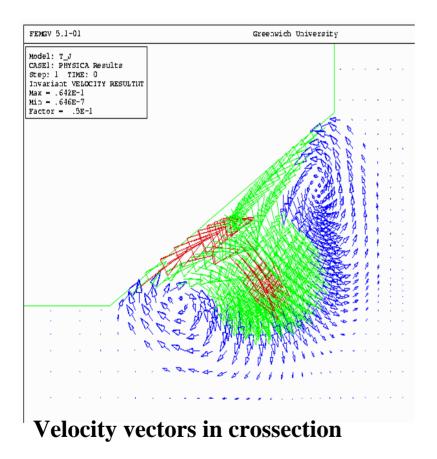
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- add to the NS momentum equations
- Extra source term in heat equation due to magnetic field | J |2 / s and include both in the CFD solution loop

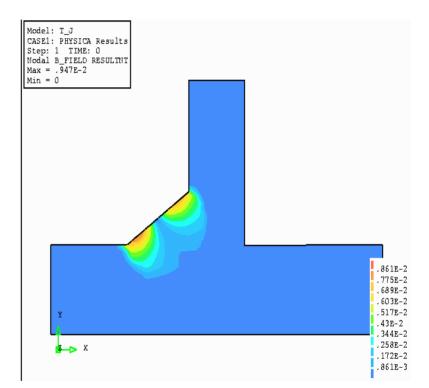




Weld Pool Dynamics



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Lorentz force distribution in the weld-pool



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Commercial Software - Electromagnetics

- General resource : http://emlib.jpl.nasa.gov/
- Vector Fields

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- http://www.vectorfields.com/
- ANSYS/EMAG
 - http://www.ansys.com/products/emag.htn
- Microstripes
 - http://www.flomerics.com/
 - Close links to Flotherm
- FLO/EMC
 - For Electronic enclosures
 - http://www.flomerics.com/



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Computational Solid Mechanics

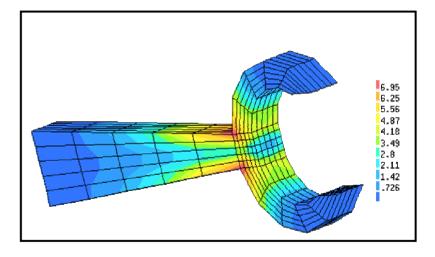
- Early work : Finite Difference
 - Simple shapes.

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- Finite Elements introduced in late 50's
 - Restricted to linear problems
 - Structural elements (beams, Trusses)
- Continuum elements introduced mid 60's
- Plasticity included in early 70's
- Finite Volume Methods now also being used (early 90's)









$$\frac{\partial}{\partial t} \left(\rho \frac{\partial u_i}{\partial t} \right) = \frac{\partial \sigma_{ij}}{\partial x_j} \qquad \sigma_{ij} = 2\mu \varepsilon_{ij}^{el} + \lambda \varepsilon_{kk}^{el} \delta_{ij} \qquad \varepsilon_{ij}^{tot} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \\ \varepsilon_{ij}^{el} = \varepsilon_{ij}^{tot} - \varepsilon_{ij}^{th} \qquad \varepsilon_{ij}^{th} = \alpha \Delta T \delta_{ij}$$

Typically

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- **Uses the Finite Element Method**
- Lagrangian Approach (Mesh moves with material)
- **Elastic material => linear,**
- **Plasticity => some non-linearity**

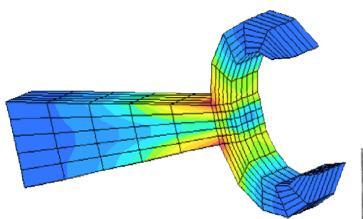




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Stress - Displacement







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Fatigue



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Commercial Software – Stress Analysis

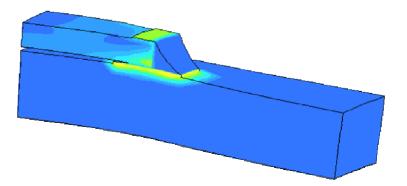
Resources at :

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http://www.engr.usask.ca/~macphed/finite/fe_resources/fe_resources.html

- ANSYS
 - http://www.ansys.com/
- MARC
 - http://www.marc.com/
- NASTRAN
 - http://www.mscsoftware.com/
- ABAQUS
 - http://www.abaqus.com









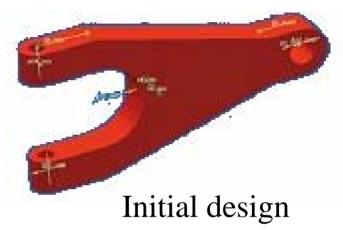


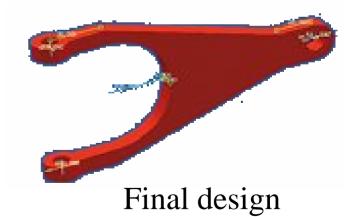
Optimisation Techniques

• Numerical

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- Design of Experiments (DOE)
- Numerical
 - Exact
 - Slow
- DOE
 - Approximate
 - Fast









Optimisation Tools

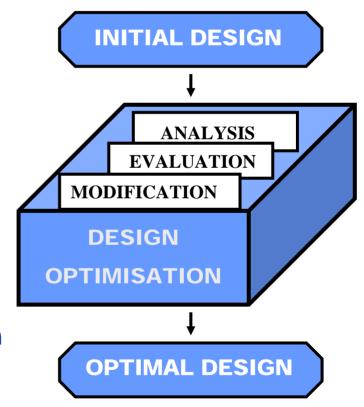
- http://optimal.hypermart.net/OPTM00.htm
- Optimisation Tool (DOT)
 - VanderPlatts

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- VisualDoc (Graphical version)
- Flexible software
- Links to Analysis codes
- http://www.vrand.com/

OptiStruct

- Altair Engineering
- http://www.altair.com/
- Structural Optimisation
- Most major CAE tools have their own optimisation modules (e.g. ANSYS)





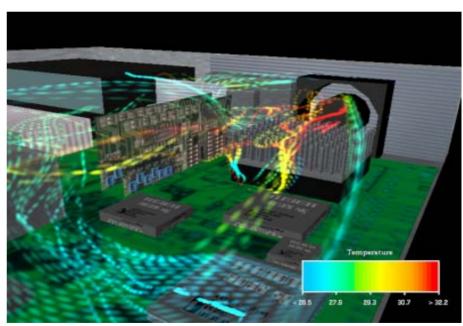




- Resource http://www.roe.ac.uk/~acd/vissys/
- Note that all analysis codes will have some visualisation capabilities.
- Leading-edge visualisation codes:
 - Wavefront

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- http://www.aliaswavefront.com/
- AVS
 - http://www.avs.com/
- Ensight
 - http://www.ceintl.com/

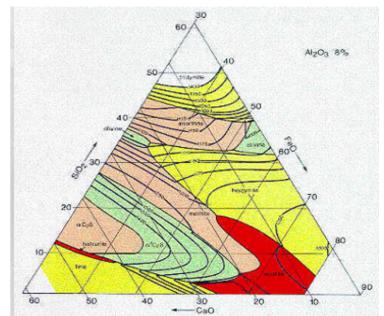






Thermodynamics Software

- Computational Thermodynamics + Databases
- Chemical and Phase equilibrium
- Function of composition and process conditions
- Can link to Macro-Models
 - i.e solidification



Software

• MTDATA

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- http://www.npl.co.uk/npl/cmmt/mtdata/mtdata.html
- Thermo-Calc
 - http://www.thermocalc.se







Multi-Physics and Multi-scale Modelling



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Story So Far

- Computational Fluid Dynamics (CFD)
- Finite Elements Computational Solid Mechanics (CSM)
- Electro-Magnetics + Magneto-Hydro-Dynamics
- Each subject solves its own set of equations for the quantities of interest (e.g. velocity, stress, current).
- Some cross over in the quantities solved for (e.g. temperature)



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We asked some people this question.. "H aving seen such a phenomenal growth in Finite Elements over the last 30 years, what do you foresee as the next giant leap in Engineering Simulation?"

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Simulatin of multiphysic & coupled phenomena. Application to health sciences and analysis and design of materials at the molecular level Roland Glowinski University of Houston



Multi-scale modelling and computing. Multi-physics and coupled phenomena. as well as uncertainty.

> H. Matthiej University of Brainaschweig



Fluid structure interaction.

Mike Chrisfield Imperial College

BAF System

Multi-disciplinary applications - much more wide spread. No more single topics, its time to look at things as a whole. Paul Dext



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Why Multi-physics Modelling ?

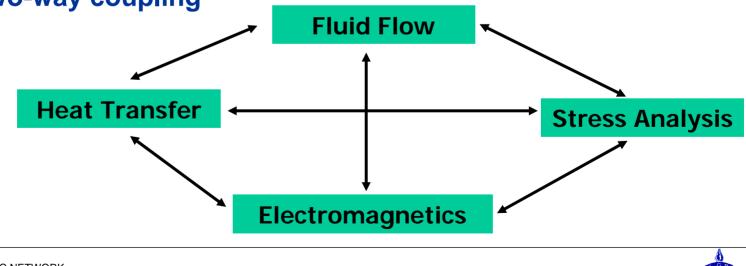
 Large number of real world problems require multiphysics simulation tools.

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• Examples

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- Solidification problems Solder Joints
- Fluid-Structure interaction Flutter in aircraft wings
- Need to solve for integrated physics
- Ensure two-way coupling



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Multi-physics Modelling

Current modelling technology mainly focused on distinct physics

- CFD (Fluid Flow)
- CSM (Stress)

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• CEM (Electromagnetics)

Multi-physics modelling

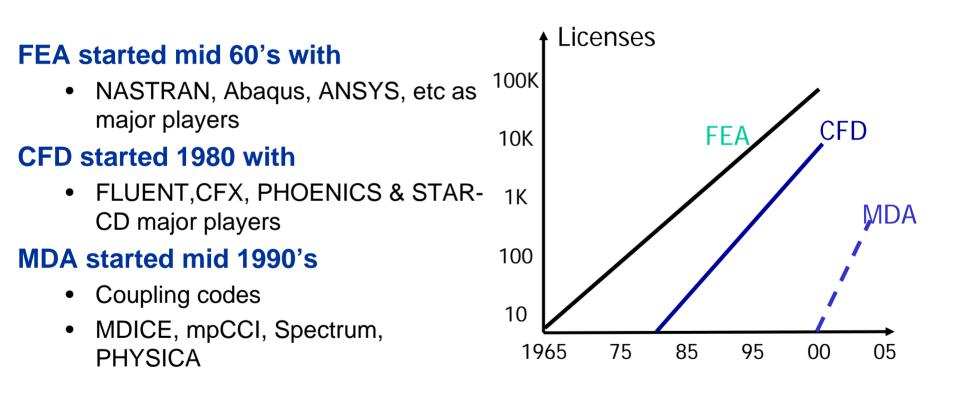
- Interface codes together: CFX ANSYS.
- Single modelling frameworks evolving.

Discretisation + Solution Procedure ?





CAE analysis tools market history





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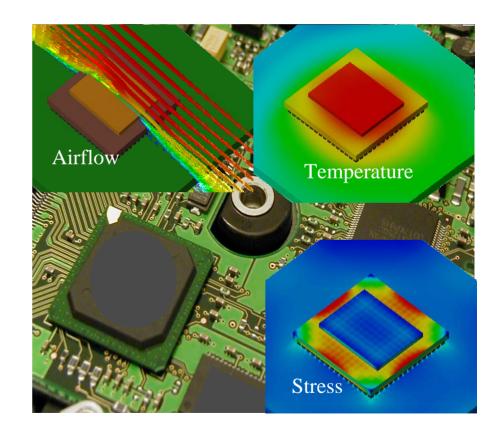
Commercial Software – Multi-physics

Number of products claiming to be multi-physics:

• ANSYS/Multi-physics

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- http://www.ansys.com/
- PHYSICA
 - http://www.multi-physics.com/
- FEMLAB
 - http://www.femlab.com/
- ADINA
 - http://www.adina.com/
- AUTODYN, etc
 - http://www.centdyn.com/
- RADIOSS
 - http://www.radioss.com/
- DYTRAN
 - http://www.mscsoftware.com/
- Algor
 - http://www.algor.com/





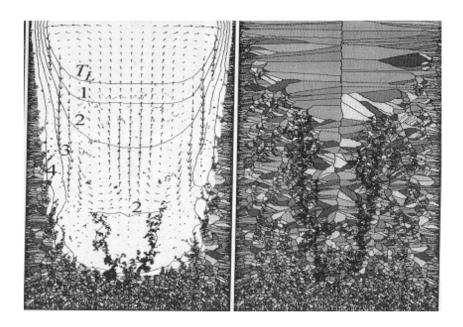




 Material performance will be governed by its microstructure

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- Nucleation and grain growth dependent on process conditions (Temperature, etc)
- Need to couple Macro Micro codes



Micro-Macro Simulation

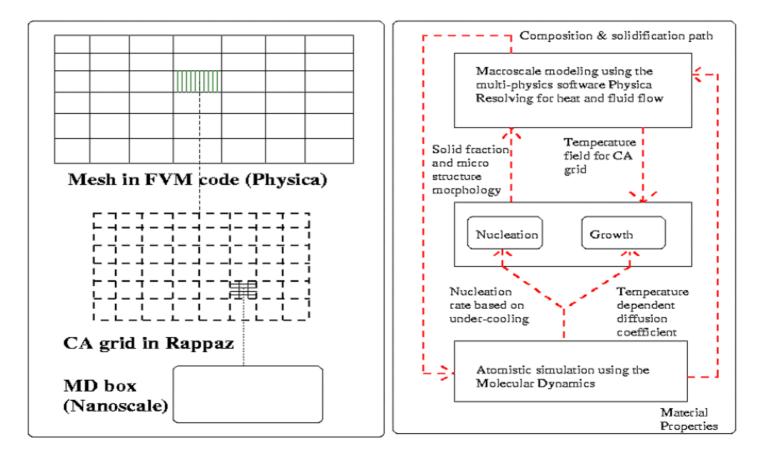
(From Ch.-A Gandin et-al, MCWASP VIII, Pub TMS (1998)



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Macro – Structure including Nano Modelling





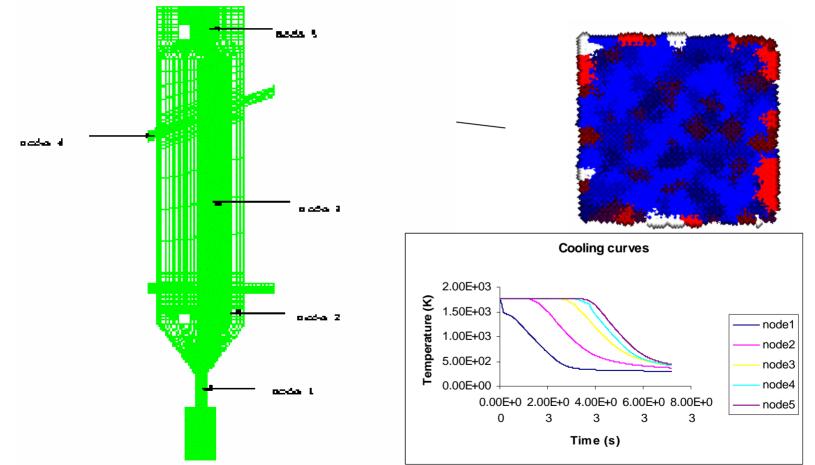
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Definition of Multi-physics Modelling

- Ask any software vendor to define what a multi-physics code is able to do:
- Ask any software vendor to define what a multi-physics code is able to do:

And most will describe their code





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Multi-physics modelling – a definition

- Definition of a multi phenomena problem:
 - A problem that requires the solution of two or more variables whose evolution is described by different classes of equations.
- For the problem to require *multi-physics* modelling there must be two way coupling between the constituent physics.
- If there is only one way coupling then the problem is *multi-disciplinary*.





Solution of Multi-physics Problems

- Two alternative approaches for a coupled problem, e.g. fluids and structures:
- Two codes

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- e.g. Ansys (CSM) and CFX (CFD)
- linked through mpCCI
- Versus
- Single code
 - e.g. PHYSICA







Issues in Multi-physics Modelling

• Levels of coupling between constituent physics

- How do variables influence each other.
- How often do variables have to be updated

Interpolation of values between solvers

- Accuracy
- Consistency







Tacoma Narrows Bridge - serious dynamic fluid structure interaction





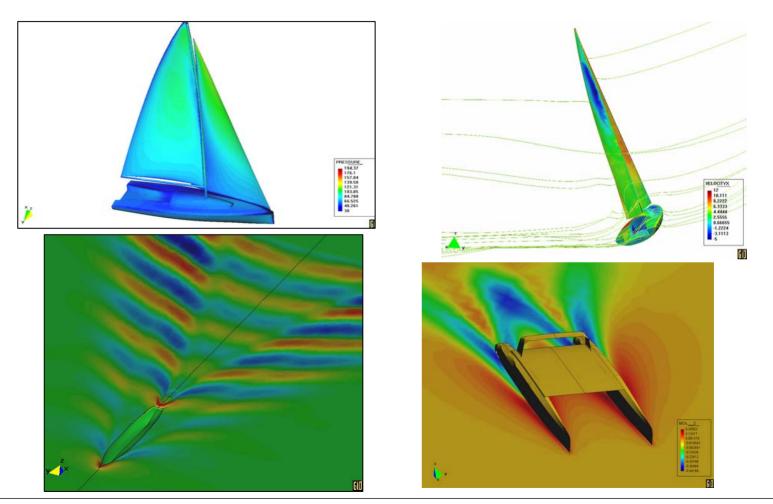


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Sail Boat – more DFSI





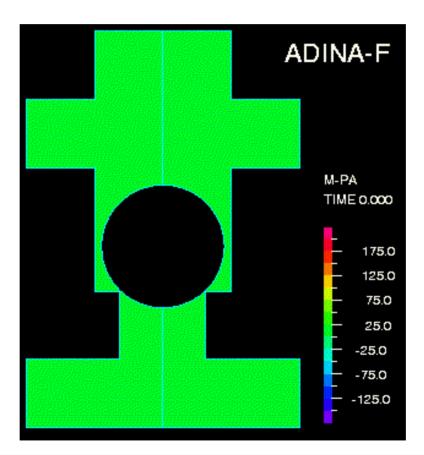
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Anti-Locking Brakes

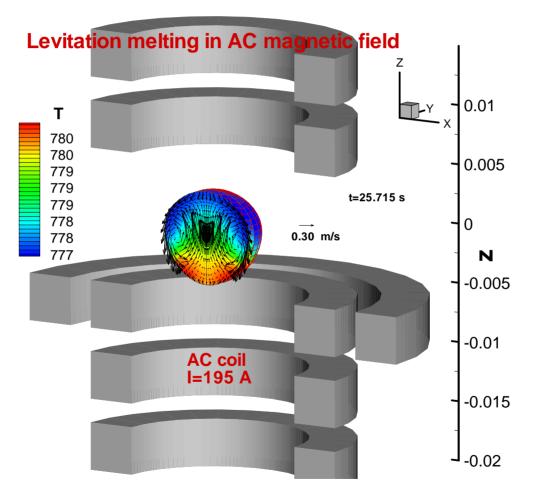




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Magnetic Levitation





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Parallel Multi-Physics Modelling



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Multi-physics simulations : compute issues

- Genuine multi-physics has many key interactions
- Macro-defects predicted as a function of these interactions
- Simulation time on Compaq Alpha can be horrendous- measured in weeks, for a problem with only 75K nodes - not practical!!!
- Conclusion can do multi-physics casting, etc simulation, but compute demand is extensive





Multi-physics compute demands:

- Unstructured Mesh analysis = 3* Structured mesh analysis
- Performance on a Compaq alpha 466Mhz
 - Seconds per node or element per time step per problem class
 - Heat Transfer (HT) + Solidification (Sol) = 2. 10-3
 - Fluid Flow (FF) + HT + Sol = 6.10-3
 - HT + Sol + Stress = .09/ .55
 - FF + HT + Sol + Stress = .14
- Casting simulation with 100K nodes, and 100 time steps is in excess of 300hours!
- Need simulation times that are 10-20x faster
- PARALLEL WITH CHANGING PHYSICS

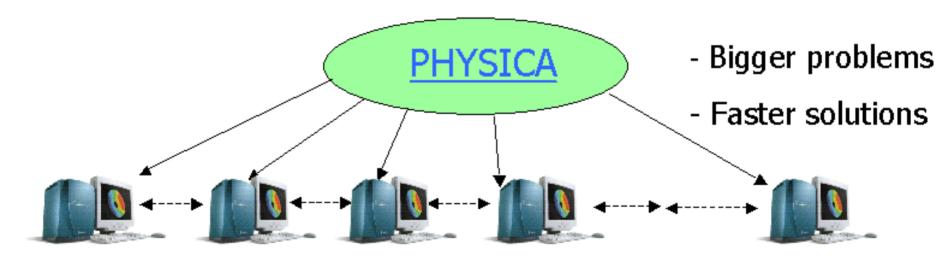






Parallel Strategy

- Single Program Multiple Data (SPMD)
- Program resident on each processor
- Mesh Partitioned across processors.
- Minimise communication times.





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- Partition of 3D unstructured mesh by JOSTLE assuming a non- homogeneous load balance across the mesh:
- SPMD Strategy

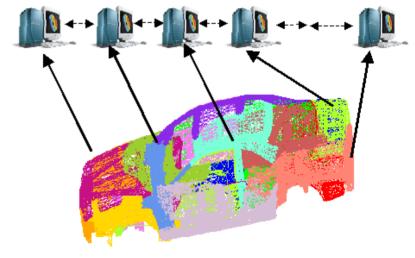
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- load balanced (even distribution per processor)
- attempts to minimises sub-domain interface elements
- sub-domain connectivity matches processor topology of the parallel system

http://www.gre.ac.uk/~jostle/







Multi-physics Simulation parallel issues

• Sub-domains have specific physics so partition must reflect this:

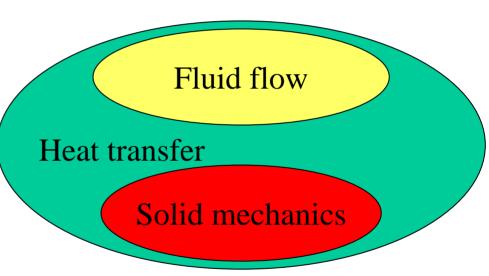
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- non-uniform load/node
- Distinct physics uses distinct discretisation procedures:
 - secondary partitions
- Also, sub-domains may change as problem develops:
 - dynamic load balance











Physics Requirements

- Fluid Flow
- Solidification
- Stress

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• Electromagnetics

Geometry

Complex

UNSTRUCTURED MESHING PARALLEL

MULTI-PHYSICS

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Large simulations



Single Software Framework

- Key route to closely coupled multi-disciplinary (multi-physics) simulation
- Basic requirements of a SSF:

- consistency of mesh for all phenomena
- compatibility in the solution approaches to each of the phenomena
- single database & memory map so that no data transfer & efficient memory use between programs
- facility to enable accurate exchange of boundary or volume sources (e.g. body force)





PHYSICA – Multi-physics Framework

- Begun in 1988 at University of Greenwich
- Used FV methods on unstructured mesh (FV-UM) using either cell centred or vertex based discretisation approaches
- Phenomena addressed:

- Fluid Flow turbulent, free surface, multi-component
- Electro-magnetics
- Heat transfer with phase change & chemical reactions
- Solid mechanics, linear, non-linear and dynamic (also in FE!)
- Prototypes moved from 2D to 3D and from scalar to parallel
- Key issue was to ensure FLOW worked well in all contexts
- Solidification processes was originally a key target





PHYSICA :

Design of a FV-UM multi-physics modelling software tool

- Framework for the solution of any coupled set of PDEs up to second order
- Design concept object oriented with reusable software modules in FORTRAN77
- Multi-level toolkit :

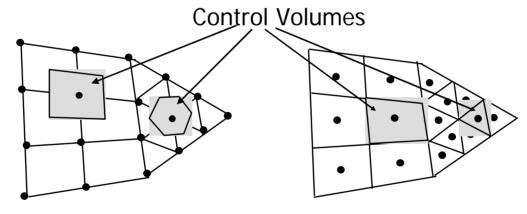
- focus at high level for model implementation
- maximise control over numerical issues
- essentially open source
- Conceived and implemented in parallel







•Uses finite volume or element procedures on unstructured mesh



Vertex-Centred Solid mechanics Cell-Centred Flow/ heat transfer

Implemented in 3D in PHYSICA



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PhD's on FV-UM techniques and tools in PHYSICA

• Chow (93) FV-UM CFD procedures in 2D

FENet

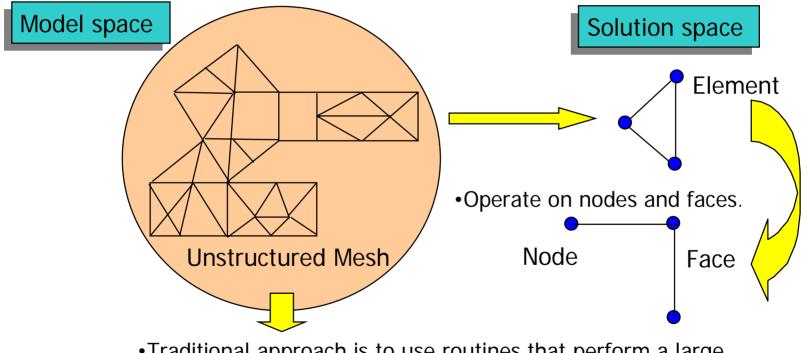
- Fryer (93) FV-UM CSM procedures in 2D
- Chan (94) FV SEA procedure in 3D free surfaces
- Hughes (94) FV-UM for MHD in 2/3D using PHOENICS
- Taylor (96) FV-UM material nonlinear CSM procedures in 3D
- McManus (96) Parallel multi-physics algorithms in 2D & 3D
- Croft (98) FV-UM CFD procedures in 3D turbulence/particle tracking/reactions
- Wheeler (00) FV-UM 3D free surfaces with surface tension and using level set
- Slone(00) FV-UM dynamic fluid-structure interaction in 3D
- Chirazi (00) FV-UM multi-scale ala Rappaz
- Fallah (01) FV-UM CSM large strain elasticity & cell centred approximations
- Edussriya (03) FV-UM non-Newtonian free surface 3D fluids
- McBride (03) FV-UM Vertex based and hybrid CFD procedures in 3D
- Stoyanov (04) FV-UM multi-physics with optimisation







Algorithms are built on methods for "Objects".



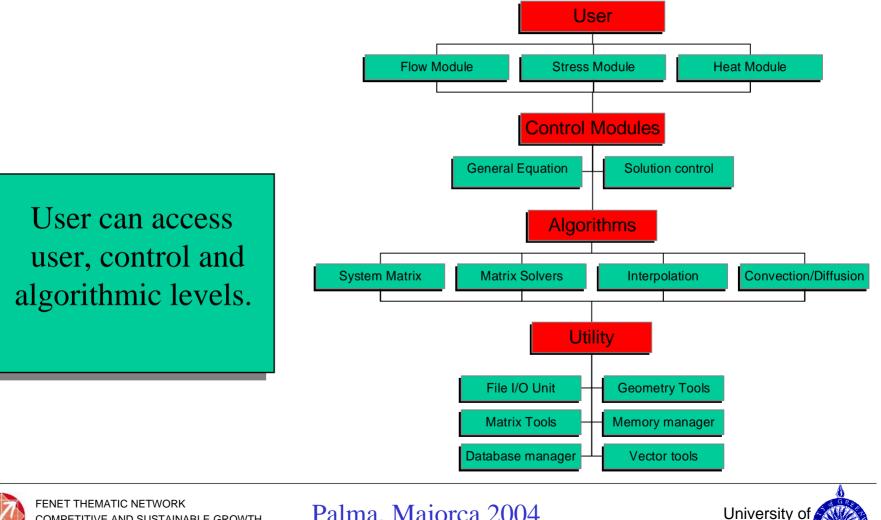
•Traditional approach is to use routines that perform a large number of operations on an element.



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Governing Equations

• The governing equations can be expressed in a standard form:

$$\frac{\partial}{\partial t}(\rho A\phi) + \nabla Q = \nabla (\Gamma \nabla \phi) + S$$

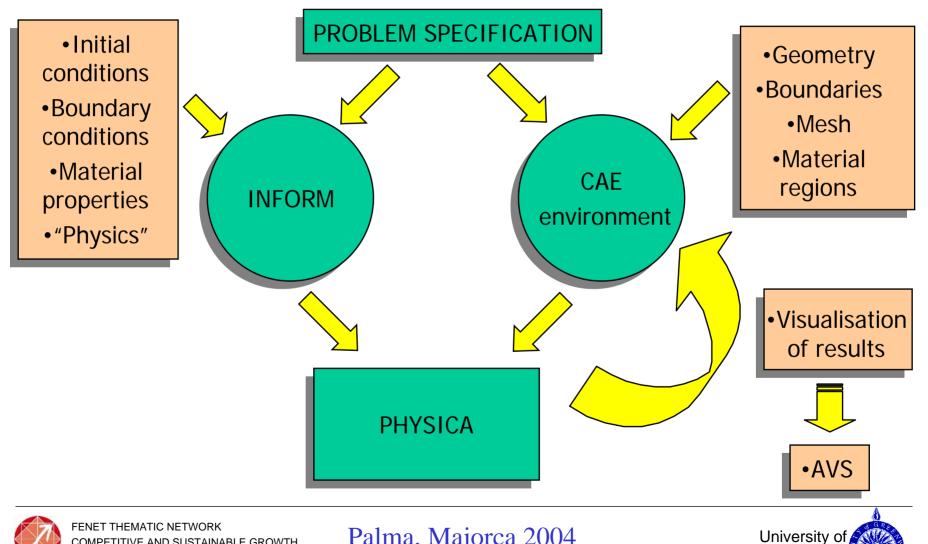
	ø	А	Γ_{ϕ}	S	Q
Continuity	1	1	0	S _{mass}	$\rho \underline{v}$
Momentum	$\underline{\mathcal{V}}$	1	Γ_{v}	$\left(S + \underline{J} x \underline{B} - \nabla P\right)$	$\rho \underline{v.v}$
Heat transfer	h	1	k/c	${S}_h$	$\rho \underline{v} h$
Electromagnetism	<u>B</u>	1	η	$(\underline{B}\nabla)\underline{v}$	<u><i>u.B</i></u>
Solid Mechanics	<u>U</u>	$\partial / \partial t$	μ	$\rho \underline{f}_b$	$\mu(\operatorname{grad} \underline{u})^{T} + \lambda(\operatorname{div} \underline{u} - (2\mu + 3\lambda)\alpha T)\underline{I}$



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PHYSICA+

• PHYSICA+ = PHYSICA + Femgv

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- Femgv is a pre and post processor
- PHYSICA is a modelling framework that can solve CFD, CSM and coupled problems.
- PHYSICA developed at Greenwich specifically to solve classes of multi-physics problems.







Course Presenters

Dr Avril Slone

- BSc (Maths) PhD (Multi-Physics)
- Senior Research Fellow, University of Greenwich
- Core development team for PHYSICA
- In another life mother of two grown up children & a Chartered Statistician.

Prof Mark Cross

- BSc (Maths) PhD (Math Physics) DSc (Comp Engg)
- Professor and Director of Centre for Numerical Modelling and Process Analysis, University of Greenwich
- Worked on Multi-Physics since inception of subject
- In another life father of 3 grown up kids and Pro Vice Chancellor for Research at Greenwich



