Challenges in the Computational Modeling of Multi-physics Processes and Systems – with a special focus on fluid-structure interaction (FSI)

June 20, 2007

Agenda

NAFEMS Multi-Physics Webinar
June 20, 2007
12:00pm EST (GMT -05:00, New York)

- **Welcome & Introduction**
  - Matthew Ladzinski, NAFEMS North American Representative
- **Challenges in the Computational Modeling of Multi-physics Processes and Systems – with a special focus on fluid-structure interaction (FSI)**
  - Dr. Mark Cross, University of Wales, Swansea
  - Dr. Avril Slone, University of Wales, Swansea
- **Q&A Session**
- **Closing**

THE INTERNATIONAL ASSOCIATION FOR THE ENGINEERING ANALYSIS COMMUNITY

An Introduction to NAFEMS

Matthew Ladzinski
NAFEMS
North American Representative

What is NAFEMS?

- NAFEMS is a not-for-profit membership association of nearly **800 companies** from all over the world.
- We are the:
  - International Association for the Engineering Analysis Community
  - Information source for the latest CAE technology developments
  - Source of Best Practice guides for the use of Analysis Technology
  - Provider of independent events where practicing Analysts exchange knowledge and experience
  - Voice of the CAE world

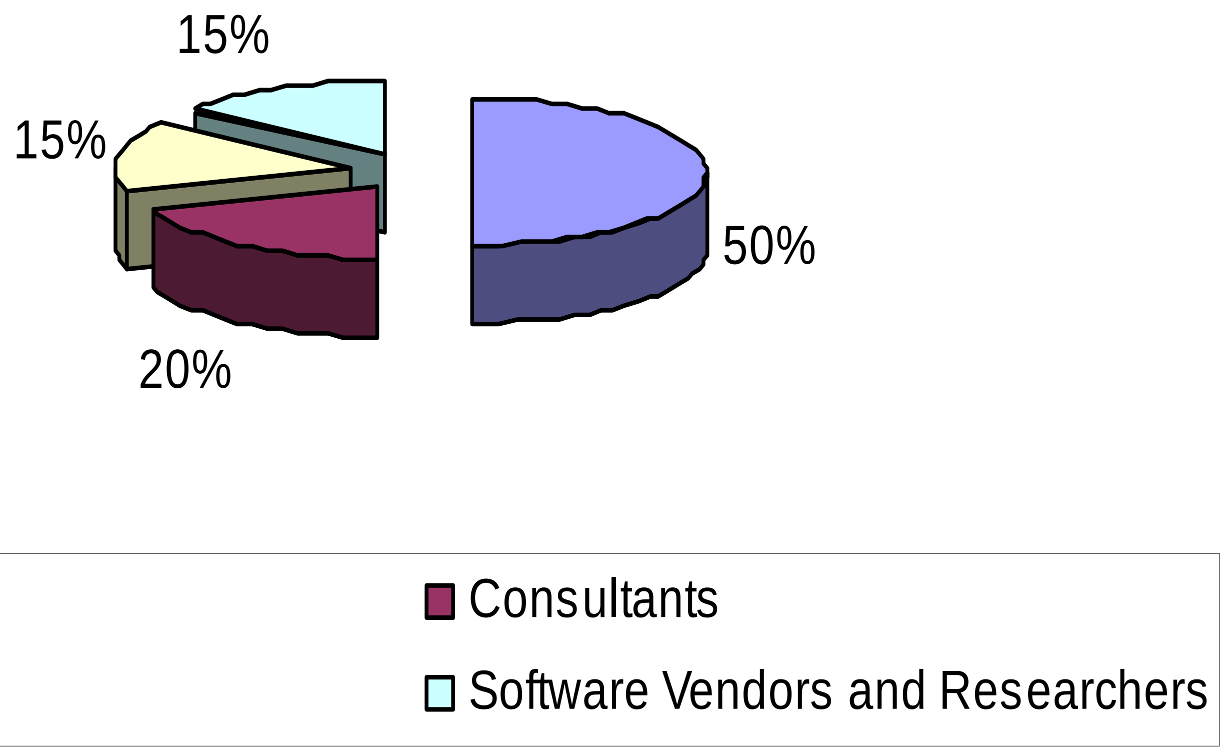
NAFEMS Objectives

NAFEMS mission is to act as a trusted source and a collaborative resource for the best engineering modeling, simulation and analysis practices in the development of safe, reliable, and affordable products. Its focus is to champion and improve best practices, to promote and enrich educational opportunities aligned with the rapidly-advancing technologies, and to advance the productivity and quality of virtual product development processes.

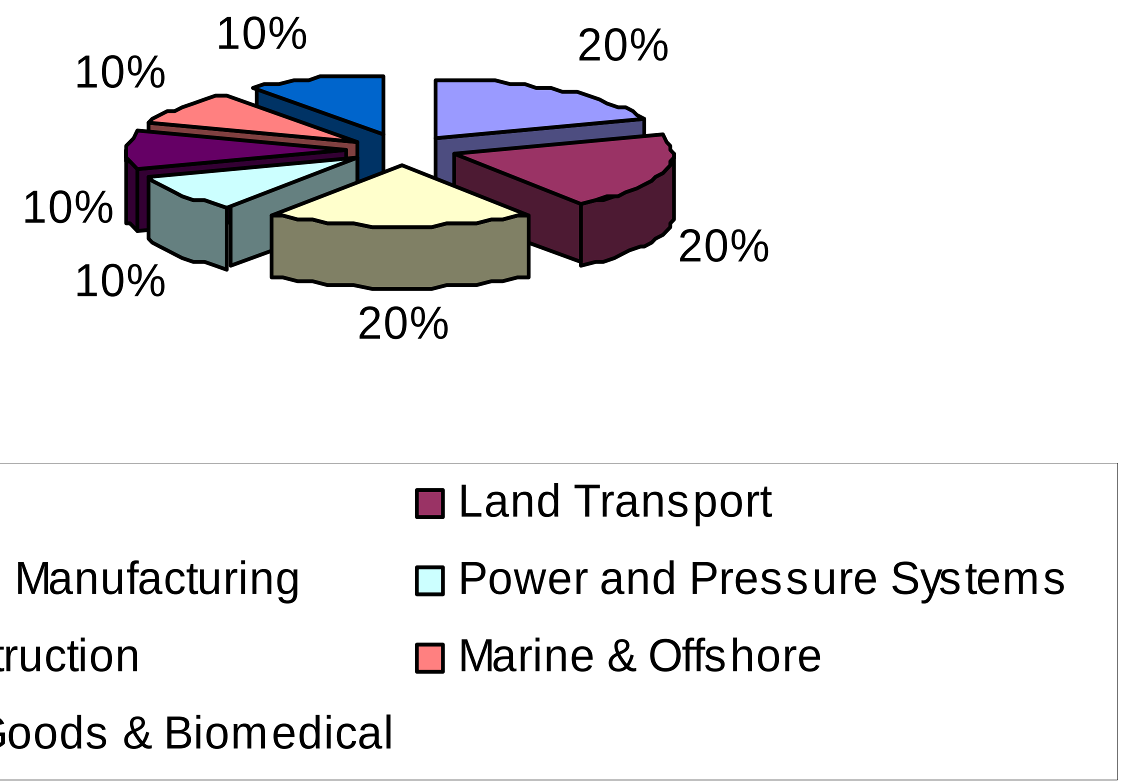
Specific objectives of NAFEMS are to:

- Promote **COLLABORATION** within the international engineering analysis and simulation community,
- Stimulate **INNOVATION** via transfer of knowledge in the use of advanced scientific, engineering and computing technologies,
- Maximize **PRODUCTIVITY** through improved best practices used in product development engineering processes,
- Implant **QUALITY** in the methods and techniques exploited by virtual product development processes.

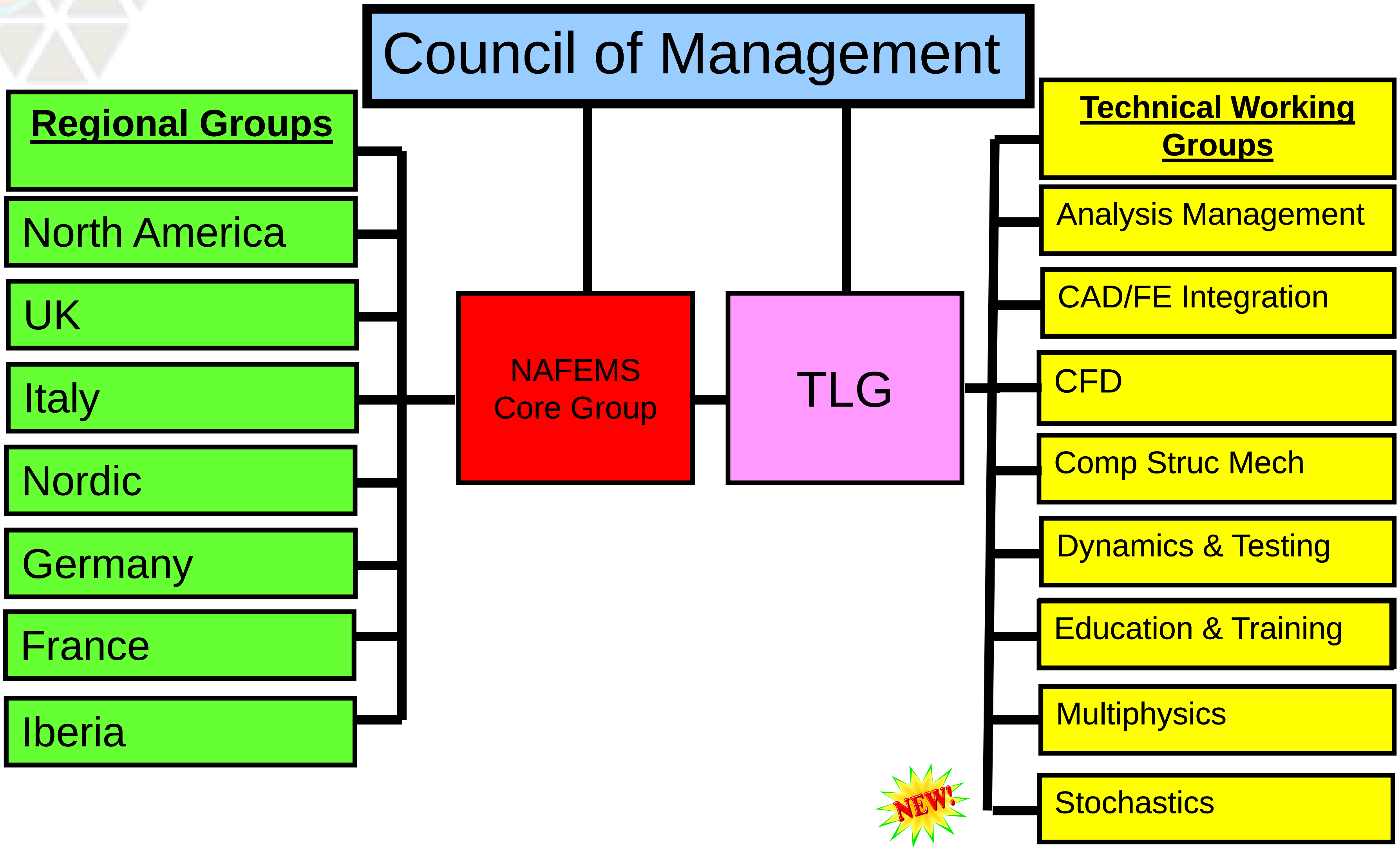
Membership Profile



Membership Profile



NAFEMS Organizational Structure



Technical Working Groups

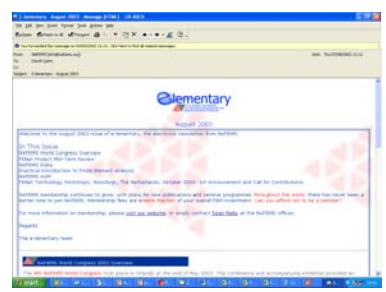
- These groups produce the NAFEMS documents (guidelines, reports, books etc.). The groups are:
  - Education & Training Working Group
  - Computational Structural Mechanics Working Group
  - CFD Working Group
  - CAD/Integration Working Group
  - Analysis Management Working Group
  - Multiphysics Working Group
  - Dynamics and Testing Working Group
  - Stochastics Working Group NEW!

Publications

Library of internationally acclaimed publications developed over the years including:

- Primers
- "How to…" Guides
- "Why do..." Guides
- Benchmarks

Issued to members as deliverables as they are developed



Planned Activities in North America

- Planning a significant increase in activities over coming months:
  - Work Session on the Management of Simulation Data
    - "***Take Control of Your Analysis and Simulation Data***"
    - September 27, 2007
    - www.nafems.org/92707
  - Webinars
    - New topic each month!
      - Process Management, July 2007
    - Recent webinars:
      - NWC07 Preview
      - Simulation-supported Decision Making
      - Simulation Driven Design (SDD) Findings
      - NAFEMS Discovery

For the latest information, please refer to the NAFEMS website:
http://www.nafems.org/regional/north_america

THE INTERNATIONAL ASSOCIATION
FOR THE ENGINEERING ANALYSIS COMMUNITY

Thank you!

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Challenges in the Computational Modeling of Multi-physics Processes and Systems – with a special focus on fluid-structure interaction (FSI)

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School of Engineering

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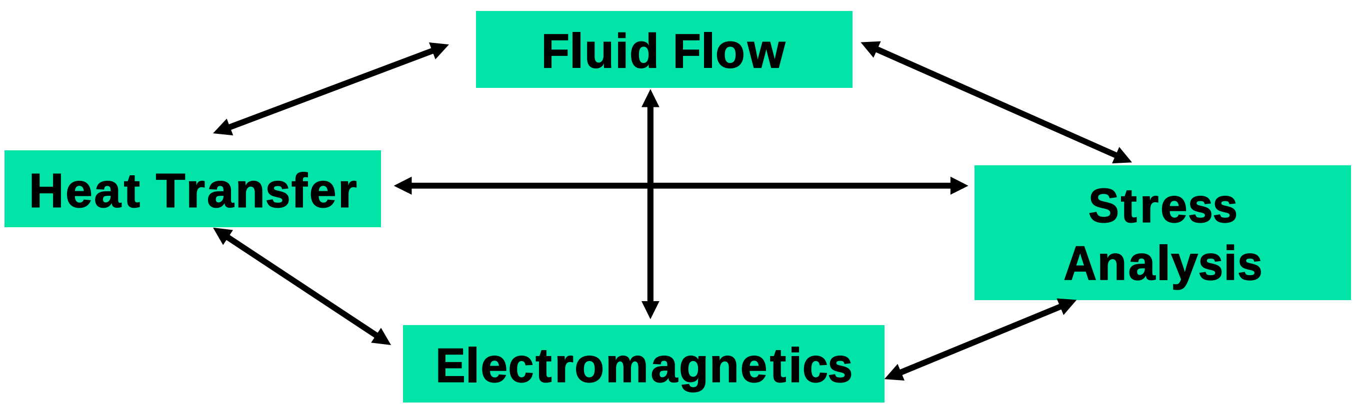
NAFEMS Webinar

June 2007

Why Multi-physics Modelling ?

- Large number of real world problems require multi-physics simulation tools.
- Examples
  - Solidification problems – Solder Joints
  - Fluid-Structure interaction – Flutter in aircraft wings
- Need to solve for integrated physics
- Ensure two-way coupling



Challenge of multi-physics

- **Multi-physics** - closely coupled interactions amongst separate continuum physics phenomena
- CAE analysis software essentially phenomena specific :
  - CFD - FV techniques with segregated iterative solvers
  - CSM - FE techniques with direct solver structure
  - CAA & CEM uses any of FE/FV/BE/FDTD techniques

  plus heritage software approaches that go with each.
- Must ensure **accurate filtering and mapping of data** for volume source and boundary data
- Must ensure that where needed, **the mesh and geometries deform compatibly**

Directly Coupled Problems

$$\underline{\mathbf{K}}\,\underline{\mathbf{a}} = \underline{\mathbf{f}}$$

$$\underline{\mathbf{K}} = \begin{bmatrix} \underline{\mathbf{K}}_f & \underline{\mathbf{K}}_{fs} & \underline{\mathbf{K}}_{ft} \\ \underline{\mathbf{K}}_{sf} & \underline{\mathbf{K}}_s & \underline{\mathbf{K}}_{st} \\ \underline{\mathbf{K}}_{tf} & \underline{\mathbf{K}}_{ts} & \underline{\mathbf{K}}_t \end{bmatrix}$$

$$\underline{\mathbf{a}} = \begin{bmatrix} \underline{\mathbf{a}}_f \\ \underline{\mathbf{a}}_s \\ \underline{\mathbf{a}}_t \end{bmatrix} \qquad \underline{\mathbf{f}} = \begin{bmatrix} \underline{\mathbf{f}}_f \\ \underline{\mathbf{f}}_s \\ \underline{\mathbf{f}}_t \end{bmatrix}$$

A single code for all phenomena
– coupling direct

Staggered Solution:

$$\underline{K}_f^n \underline{a}_f^n = \underline{f}_f^n - \underline{g}_1(\underline{a}_s^{n-1}, \underline{a}_t^{n-1})$$

$$\underline{K}_s^n \underline{a}_s^n = \underline{f}_s^n - \underline{g}_2(\underline{a}_f^{n}, \underline{a}_t^{n-1})$$

$$\underline{K}_t^n \underline{a}_t^n = \underline{f}_t^n - \underline{g}_3(\underline{a}_s^{n}, \underline{a}_t^{n})$$

Impact of using distinct solvers for each phenomenon

Explicit or implicit

Classifying multi-physics

- Most vendors advertise *multi-physics*
- Most vendors offer *multi-disciplinary*
- *Multi-disciplinary* – using data generated by one code as input into another – *loose or one way coupling*

  (e.g. electric field loading a thermal calculation)
- *Multi-physics* – two way exchange of information, which could involve implicit convergence within a time-step

  (e.g. thermo-mechanical)
- *Closely coupled multi-physics* – time and space accurate exchange of data

  (e.g. dynamic fluid-structure interaction)

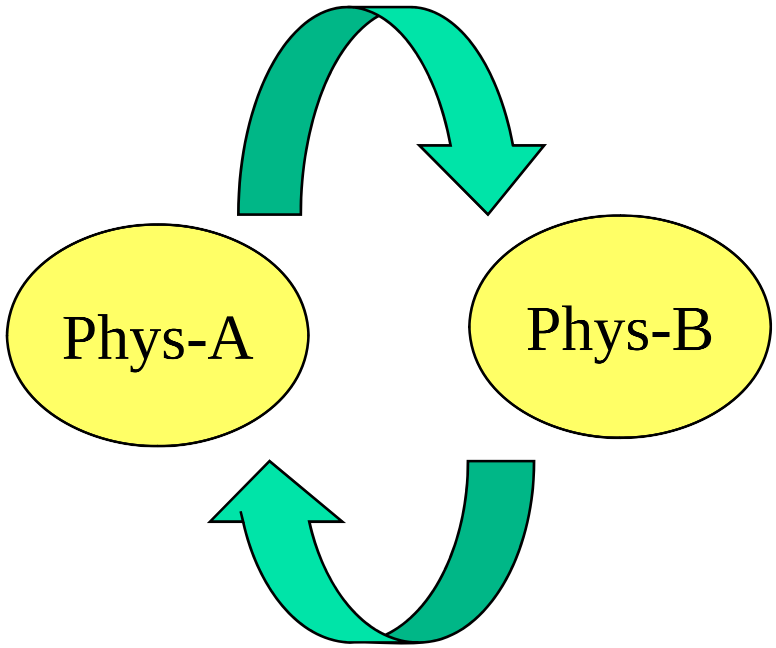
Key issues in closely coupled multi-physics simulation

- Interpolation from one set of variables to another => **compatibility of mesh**

- **Virtual single database** of mesh data & simulation variables

- **Solver strategy**
  - direct vs iterative
  - Eulerian vs Lagrangian

- Is coupling strategy compatible with **scalable parallelism**, EVEN if software components are parallel



Multi-physics: coupling issues

a) Existing 'component' phenomena analysis software – **coupling**

b) **Need a filter structure for code interoperability**:- exchange information directly from each others database **without opening closing files**

c) Options here derive from tools for developed for parallelisation – especially PVM, MPI and **specifically MpCCI**

d) **Interoperability** not equivalent to simulating physics of coupling

e) **Remaining Challenge -** parallel scalability of interoperable codes

MpCCI – a tool for code interoperability

- Emerged from an EU project – public domain OPEN SOURCE tools
- www.scai.fraunhofer.de/mpcci.0.html

- A number of MpCCI facilitated code couplings:
  - ABAQUS + FLUENT for DFSI
  - STAR-CD + NASTRAN for DFSI

- MpCCI here to stay and facilitates genuine coupling – initial experiences not trouble free, but . .

Sector Specific 'multi-physics' Software

- Castings
  - PROCAST http://www.ues-software.com
  - MAGMASOFT http://www.magmasoft.com
- Forming
  - DEFORM http://www.deform.com
  - SUPERFORGE http://www.mscsoftware.com
  - FORGE3 http://www.transvalor.com
- Polymers
  - C-Mold http://www.moldflow.com
- Joining Processes
  - SYSWELD http://www.esi-group.com
- Electronic cooling
  - Flotherm http://www.flomerics.com

Commercial CAE analysis - a web survey
Tools claiming multi-physics capabilities:

ANSYS/Multi-physics	http://www.ansys.com
ABAQUS	http://www.abaqus.com
ADINA	http://www.adina.com
ALGOR	http://www.algor.com
AUTODYN	http://centurydynamics.com
CFD-ACE	http://www.esi-group.com
DYNA	http://www.lsc.com
COMSOL	http://www.comsol.com/
LMS software	http://www.lms.com
MSC- NASTRAN	http://www.mscsoftware.com
PHYSICA+	http://www.physica.co.uk
STAR-CCM+	http://www.adapco.com

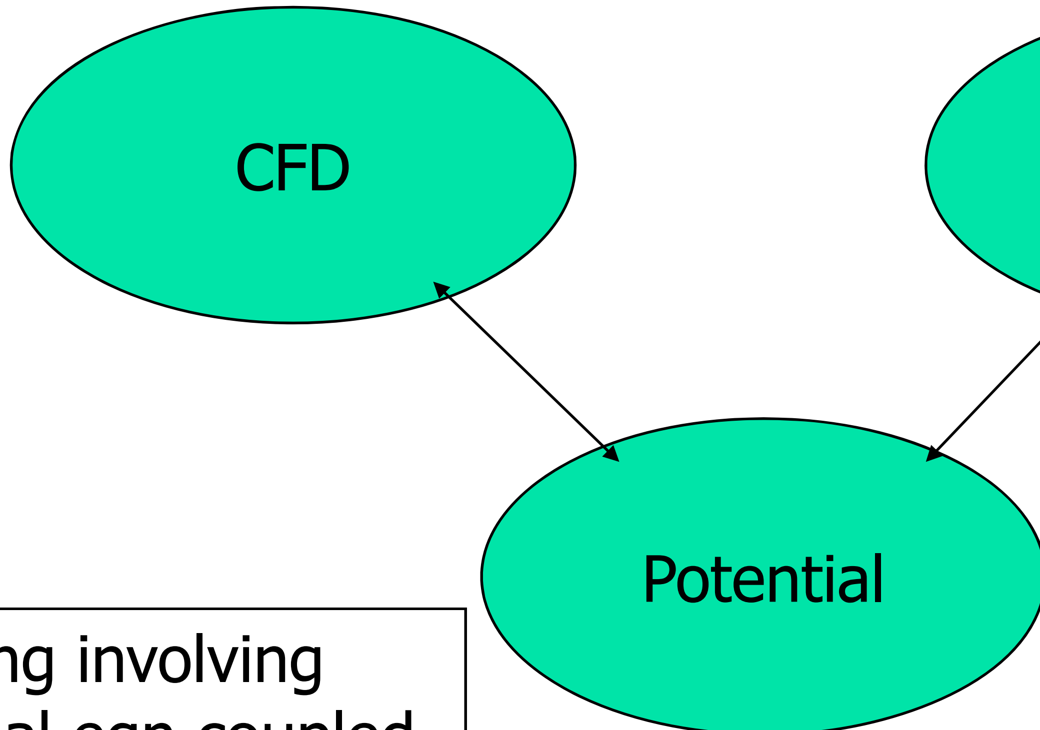
Alternative approach: Single Software Framework

- **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)
  - enables **scalable parallel operation** for all physics interactions

Single software frameworks for multi-physics

- COMSOL
  - FE solver technology with some phenomena specific modules
  - Nice environment; easy to use
- STAR-CD (& STAR-CCM+ emerging)
  - FV solver technology, polyhedral element
  - CFD based with strong meshing
- PHYSICA
  - Mixed FV (for flow, etc) & FV or FE (for stress)

'Straightforward' multi-physics

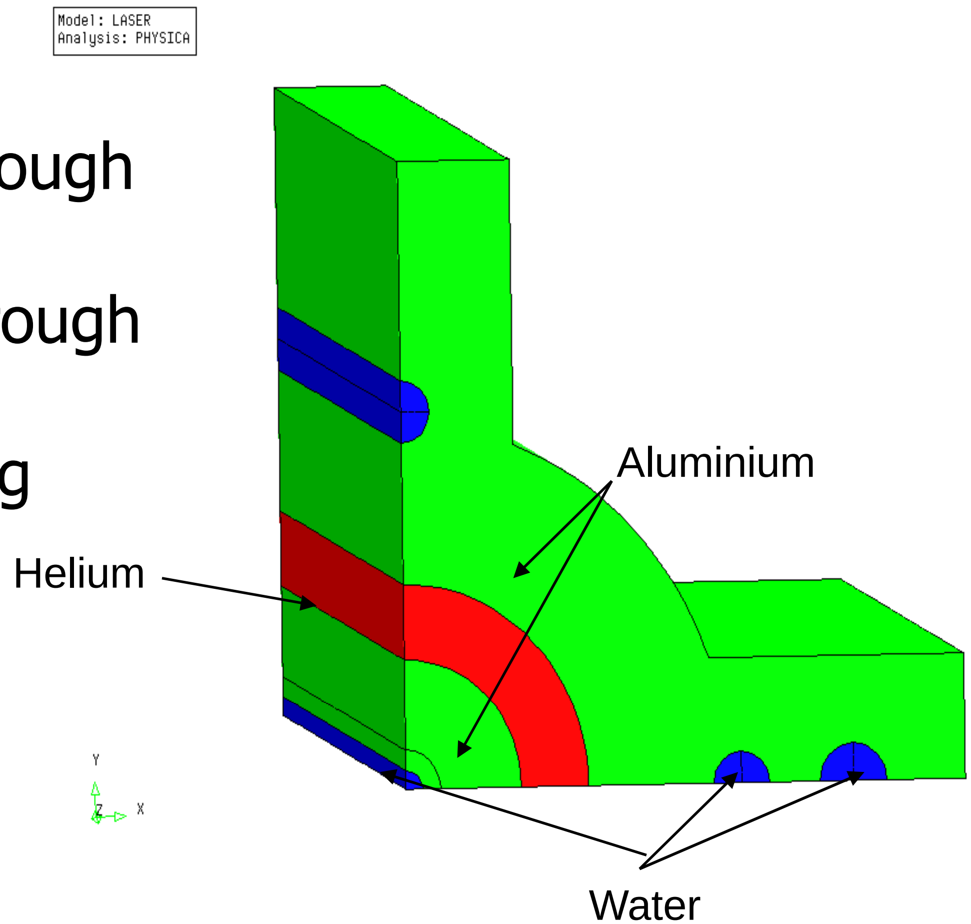


Anything involving
Potential eqn coupled
To some other physics

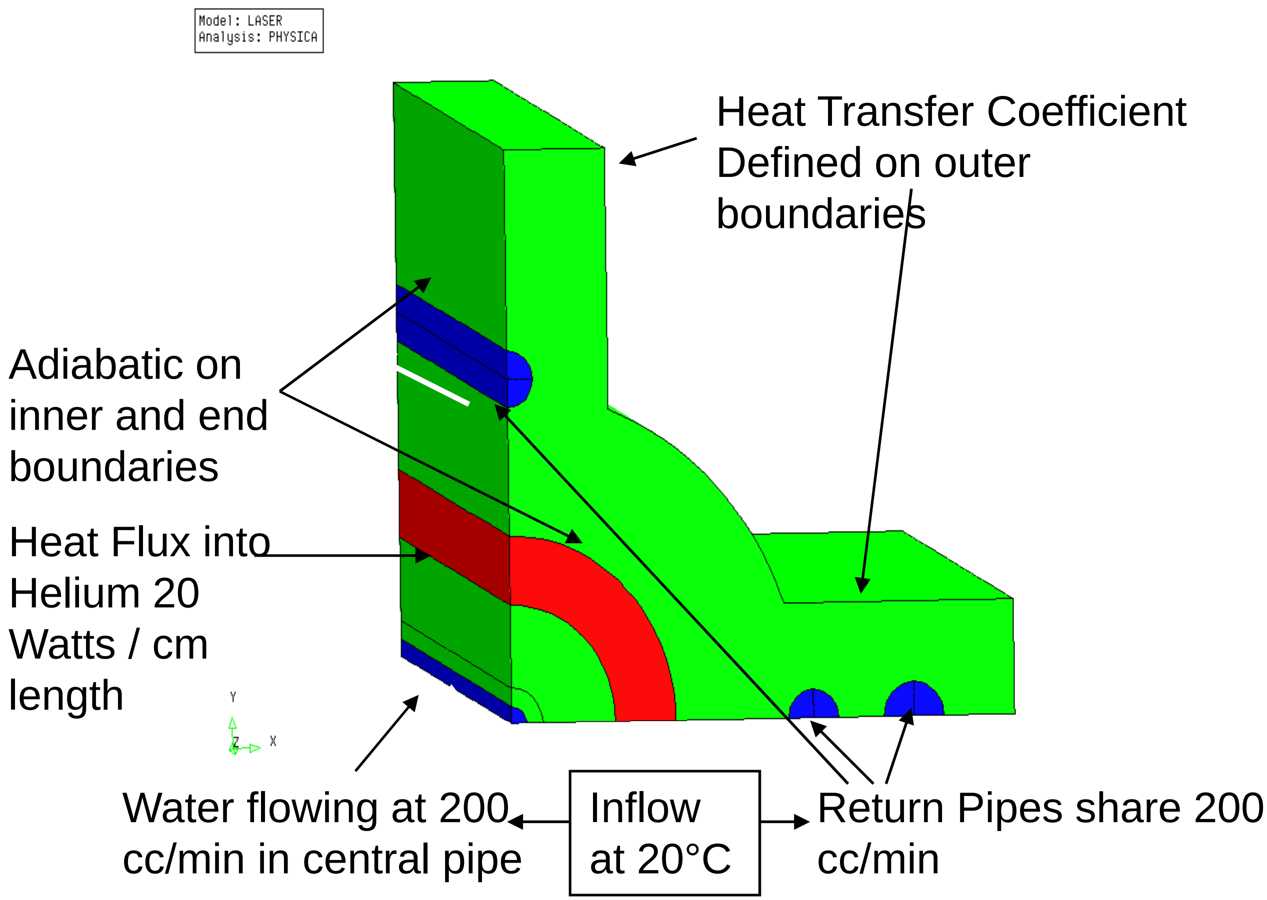
Potential eqn:
-Heat
-Electric field
-etc

Helium laser cooling system

Physics:
- Heat generation through electrical discharge
- Heat conduction through cooling system
- Flow through cooling pipes
- All coupled



Boundary Conditions

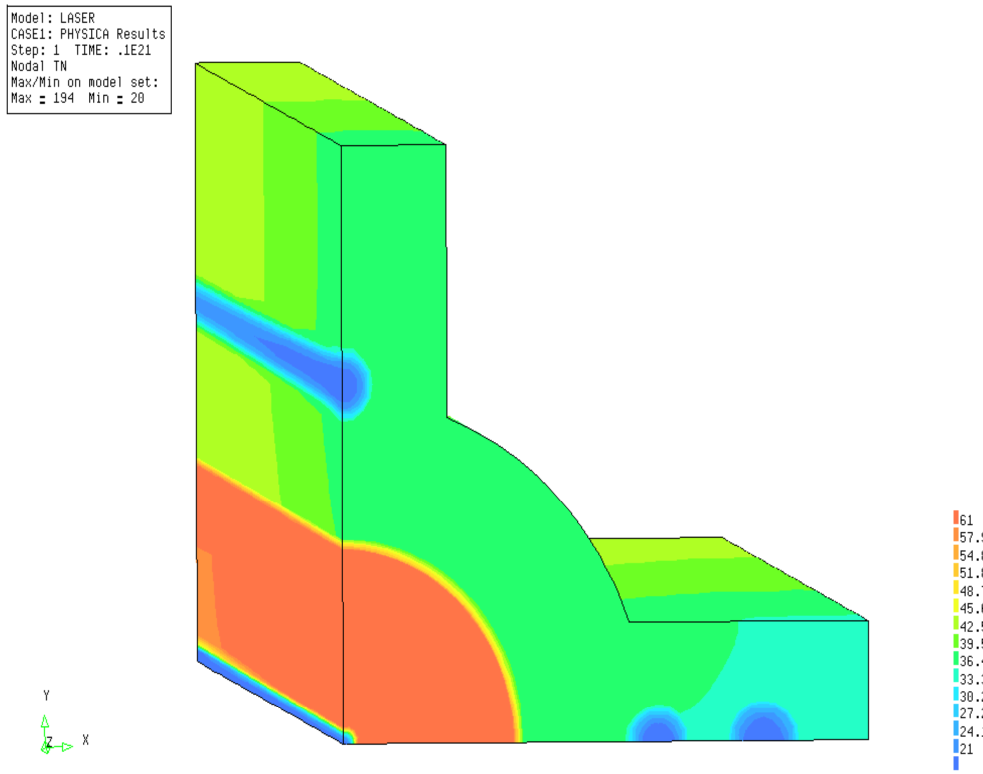


Temperature Profiles

Definitely multi-physics

BUT

straightforward



Multi-physics Modelling

- Physics Requirements
  - Fluid Flow
  - Heat transfer
  - Solidification/phase change
  - Stress
  - Electro-magnetics
  - Acoustics

→ MULTI-PHYSICS

- Geometry
  - Complex

→ UNSTRUCTURED

- Large simulations

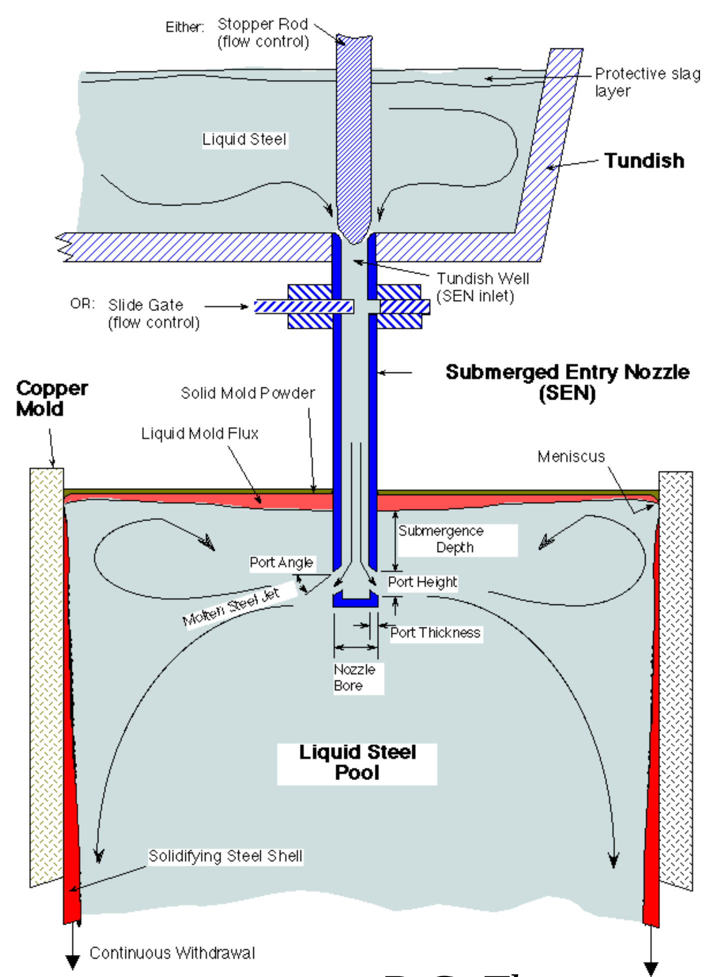
→ PARALLEL

Key issue: CFD capability

Continuous casting process: example of CFD based multi-physics

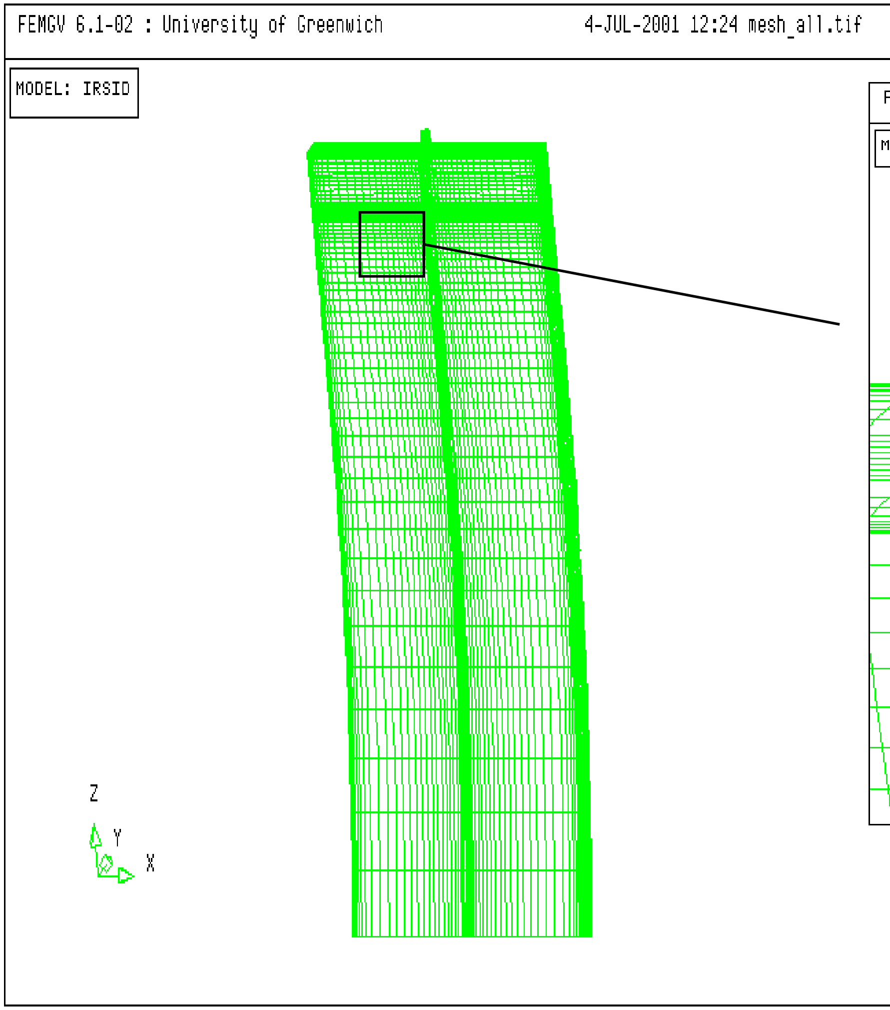
- Mixture of liquid steel and argon injected into rectangular mould
- Liquid metal flux sits on top of mould
- Water cooled mould extracts energy forming a solid steel shell
- Continuous withdrawal

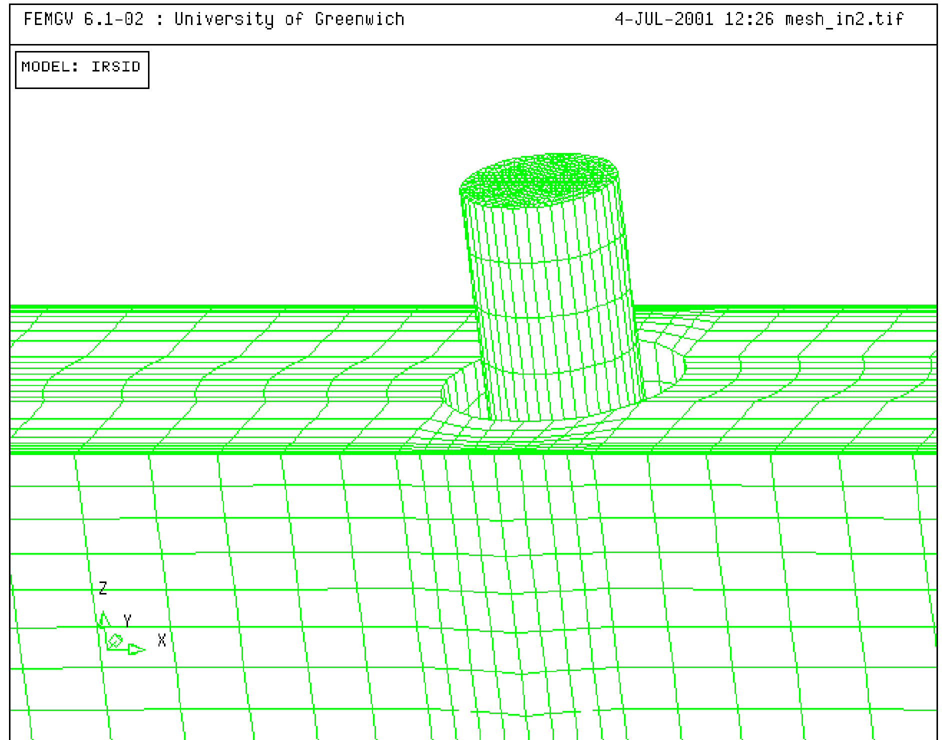
Schematic of continuous casting tundish, SEN, and mold



B.G. Thomas

Solution domain



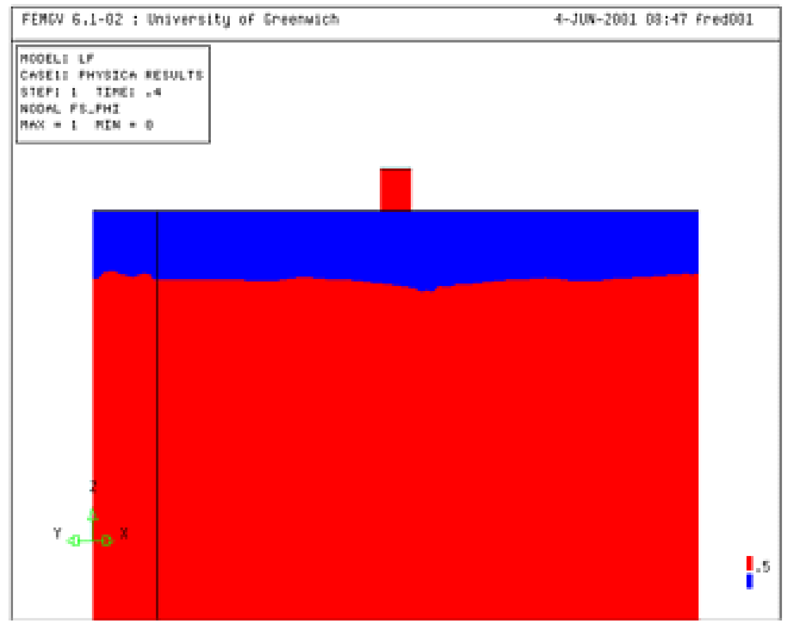


Free surface (SEA)

- **Solves:**

$$\frac{\partial \phi}{\partial t} + \mathbf{u}.\nabla \phi = 0$$

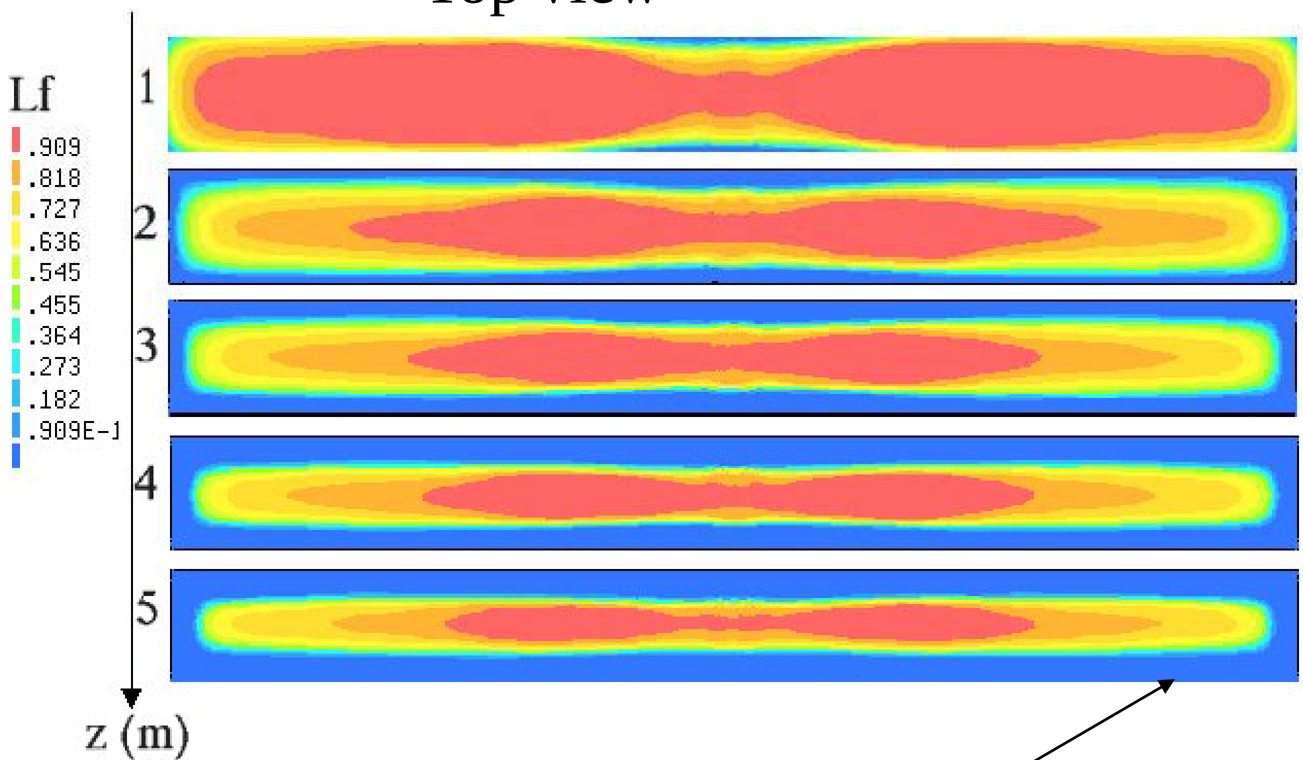
  - where ϕ is the fraction of metal in a cell

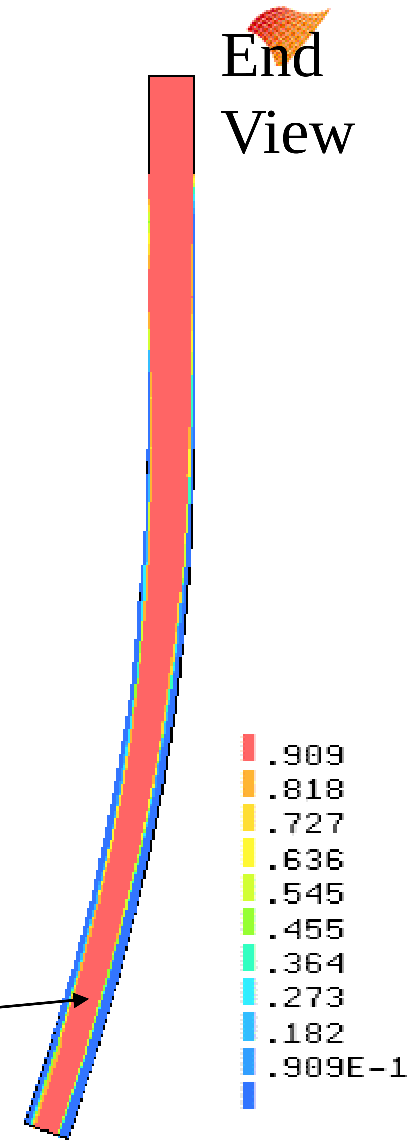


- van Leer scheme used to reduce smearing of interface
- continuity equation solved for volume not mass
- properties a linear combination of phases present

Solidification Strand

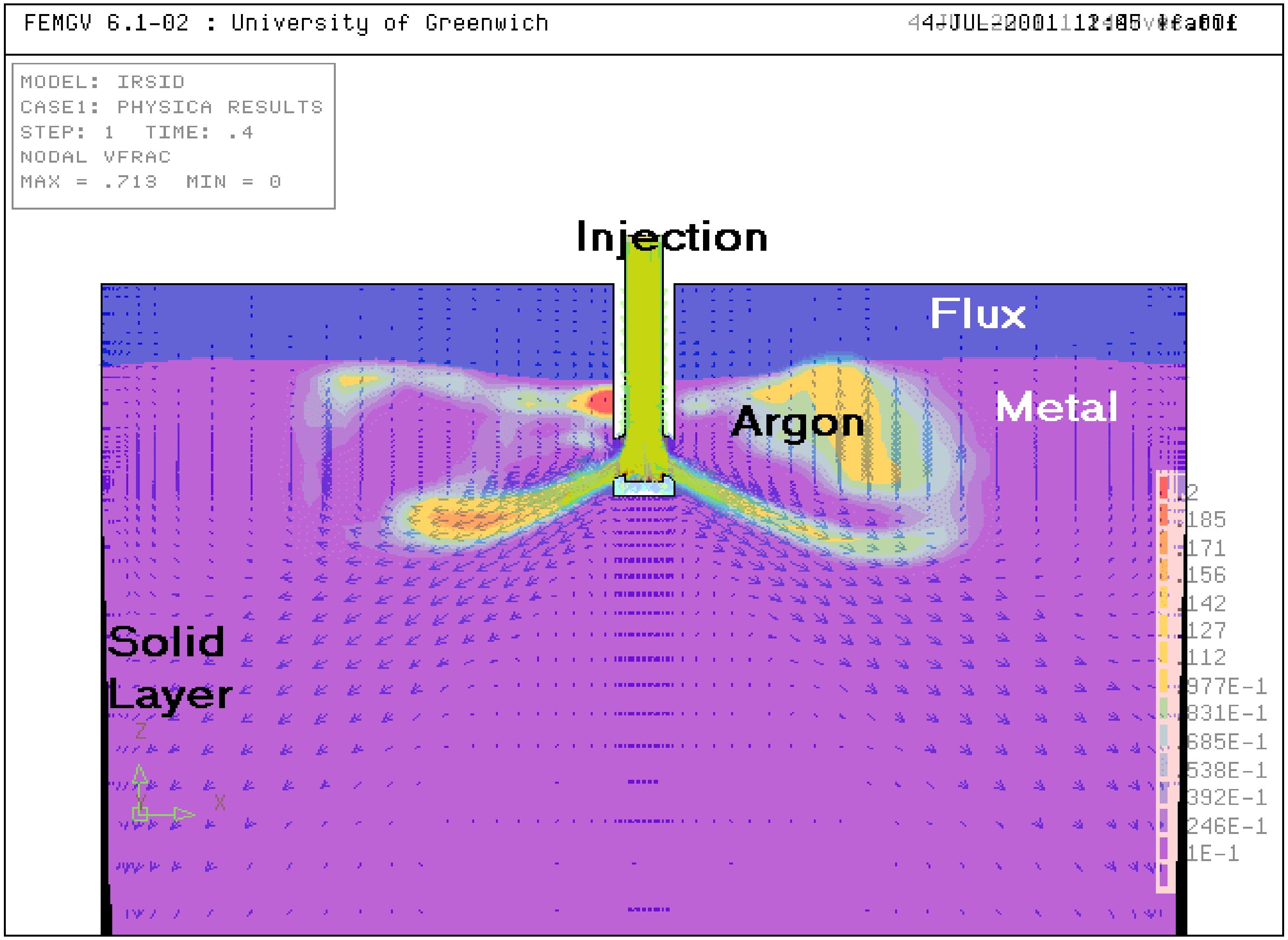
Top view





Solid regions appear in blue

Clustering of argon bubbles



Electromagnetic brake simulations

Computations were also performed to estimate the effects of EMB on the free surface . For this the Maxwell equations were solved, which with the usual MHD assumptions, lead to:

Continuity of magnetic flux: $\nabla . \underline{B} = 0$

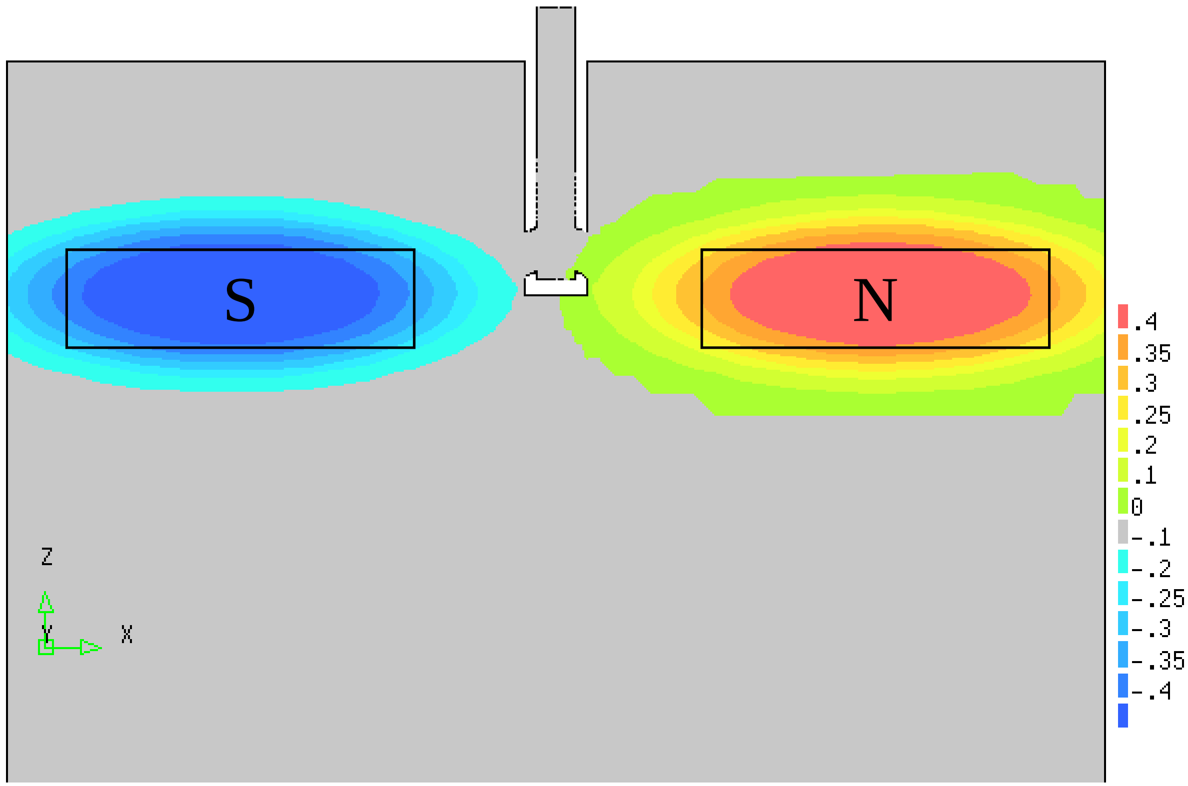
Ohm's Law for conducting metals $\underline{J} = \sigma(\underline{E} + \underline{U} \times \underline{B}),\ where\ \underline{E} = -\nabla\phi$

Magnetic Transport, or Induction equation $\frac{\partial \underline{B}}{\partial t} = \nabla \times (\underline{U} \times \underline{B}) + \eta \nabla^2 \underline{B} \quad where, \eta = \frac{1}{\sigma \mu_m}$

Lorentz force: $F_L = J \times B$

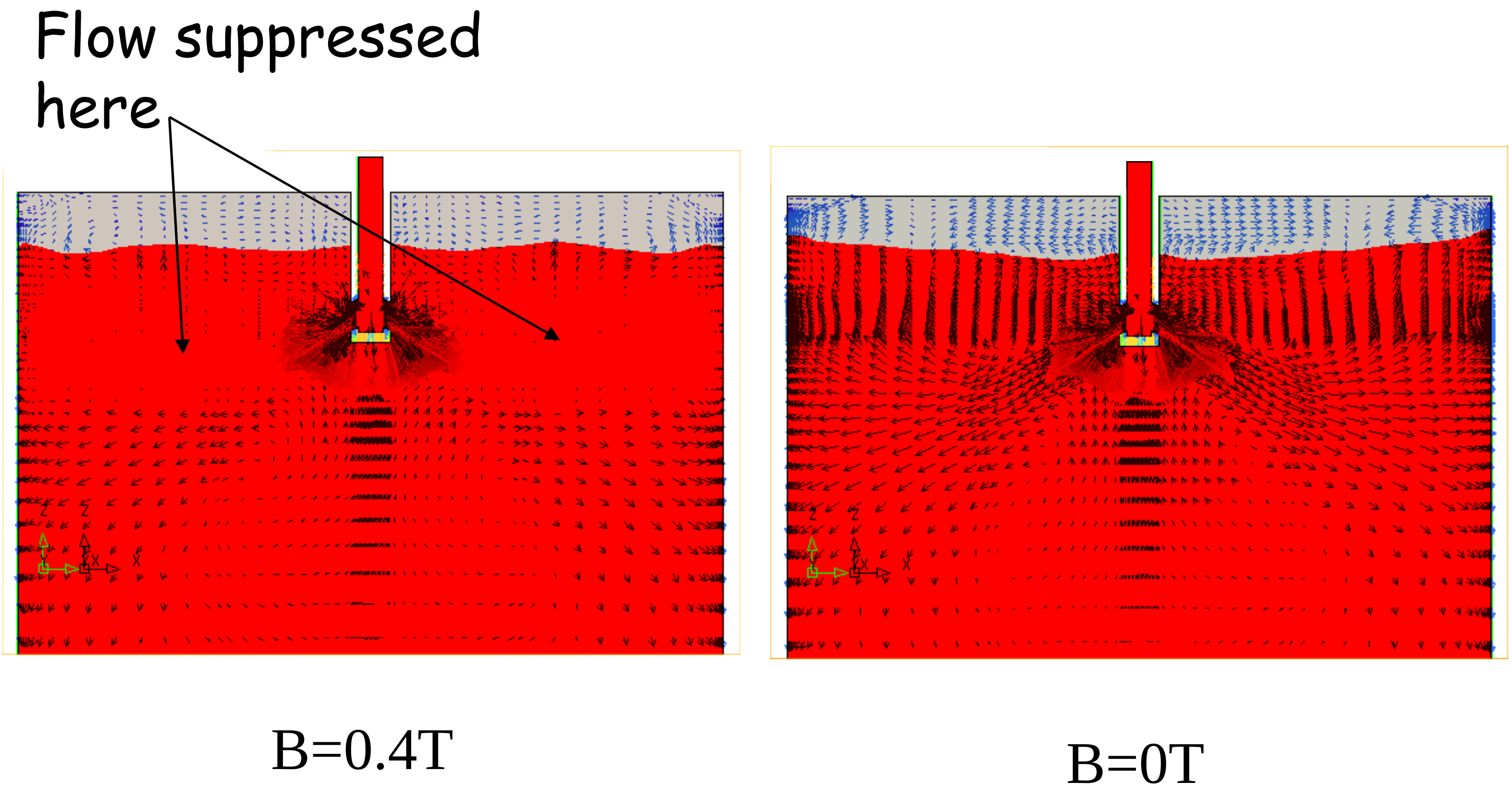
Note: Terms containing the velocity $\underline{U}$, are only important when R_m $(= LU/\eta) > 1$

Brake arrangement



Two electromagnets of opposite polarity ($B_y=\pm 0.4T$) placed in the jet region to reduce velocity and hence, surface deformation

Fluid behaviour under EMB conditions



Coupled EM-flow calculations

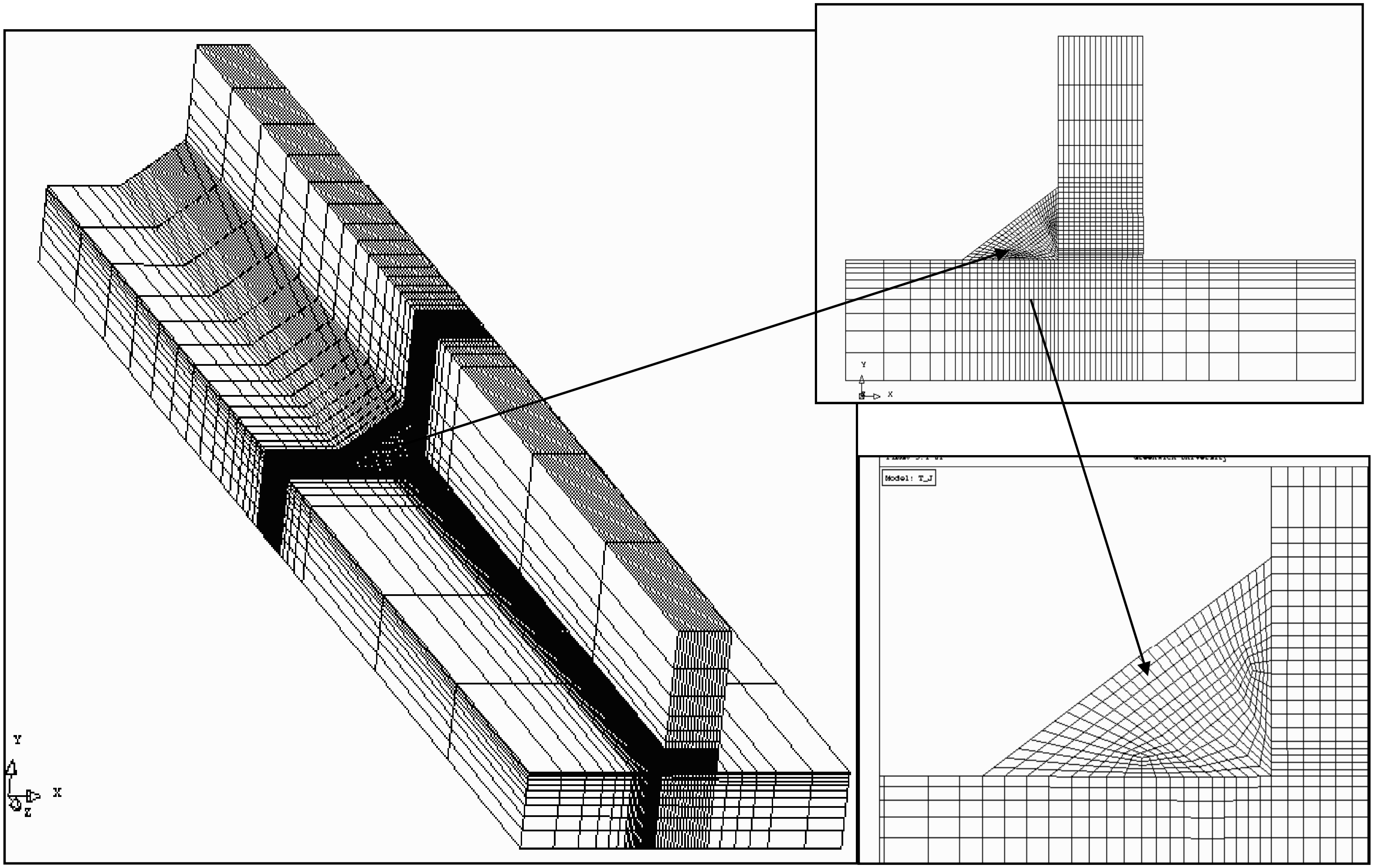
For most practical calculations in metals processing:

- The EM field influences the flow and thermal fields
- BUT the thermo-fluid phenomena has little influence of the EM fields
- Hence, essentially one way coupling
- So calculate the EM field and calculate the thermal and flow loads in the CFD calculation
- Can implement above model in any good CFD code!

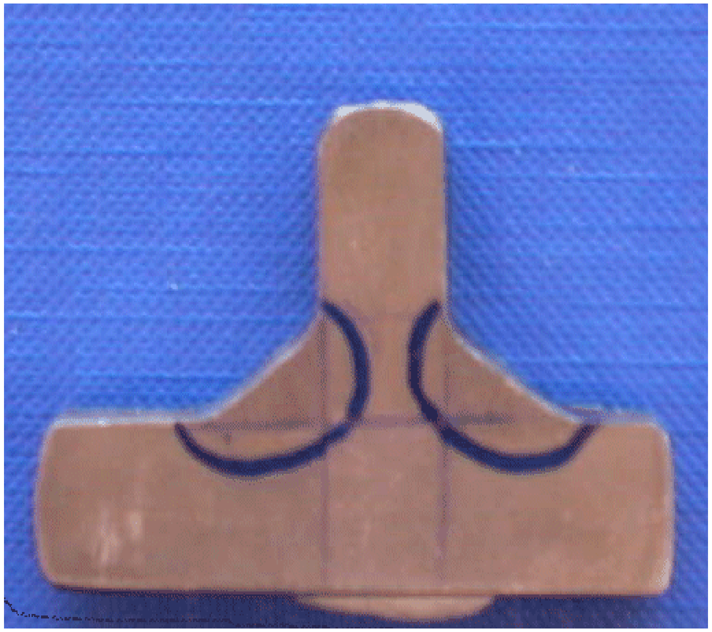
Welding processes simulation - natural multi-physics

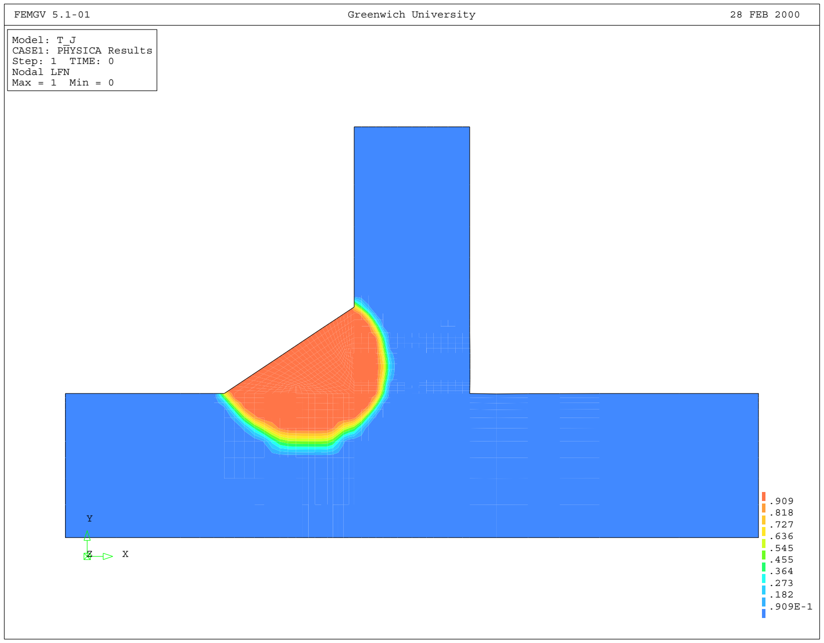
- Processes involve:
  - free surface flow
  - electromagnetic forces
  - heat transfer with solidification/melting
  - development of non-linear stress
- Ideal candidate for multi-physics modelling

T-Junction arc weld simulation



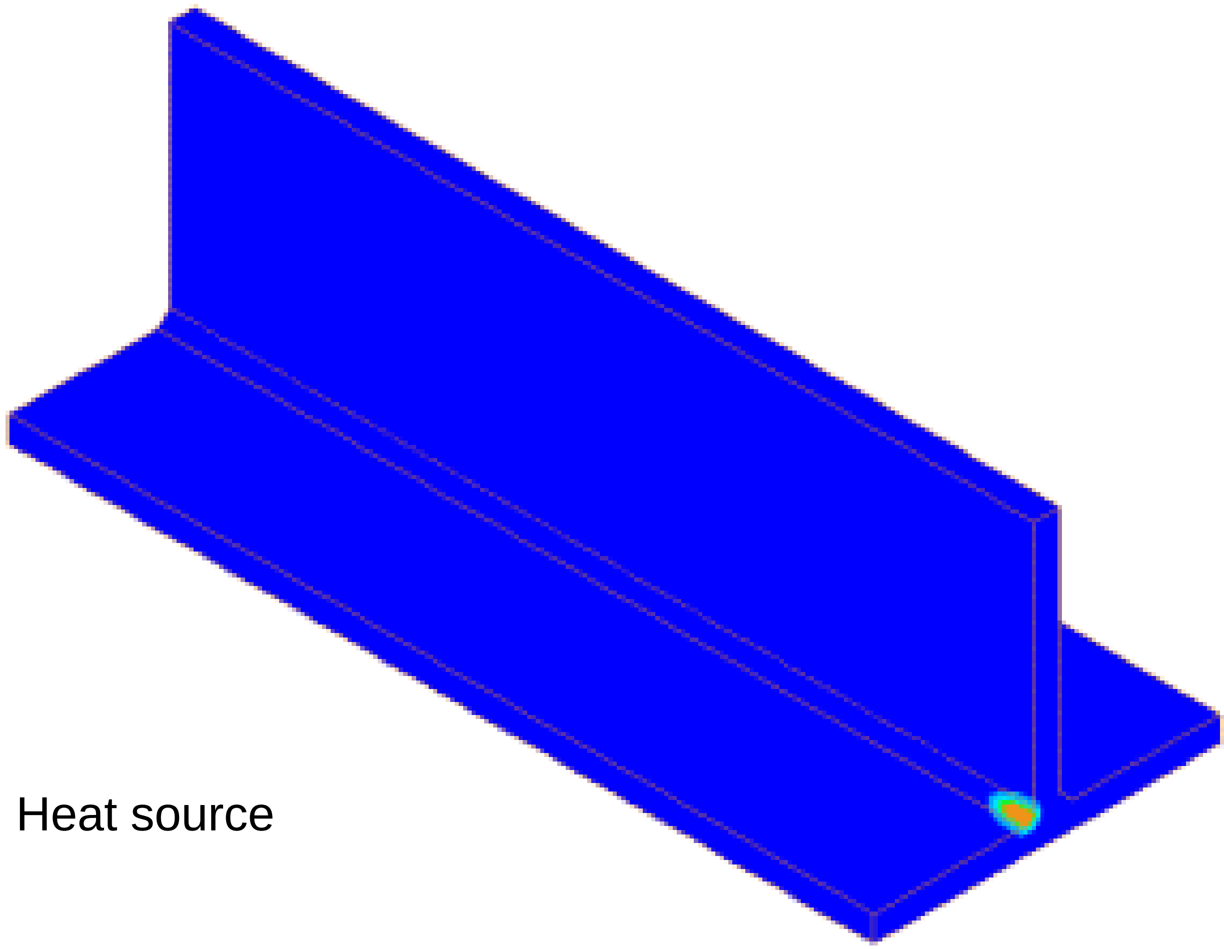
Experiment and simulation





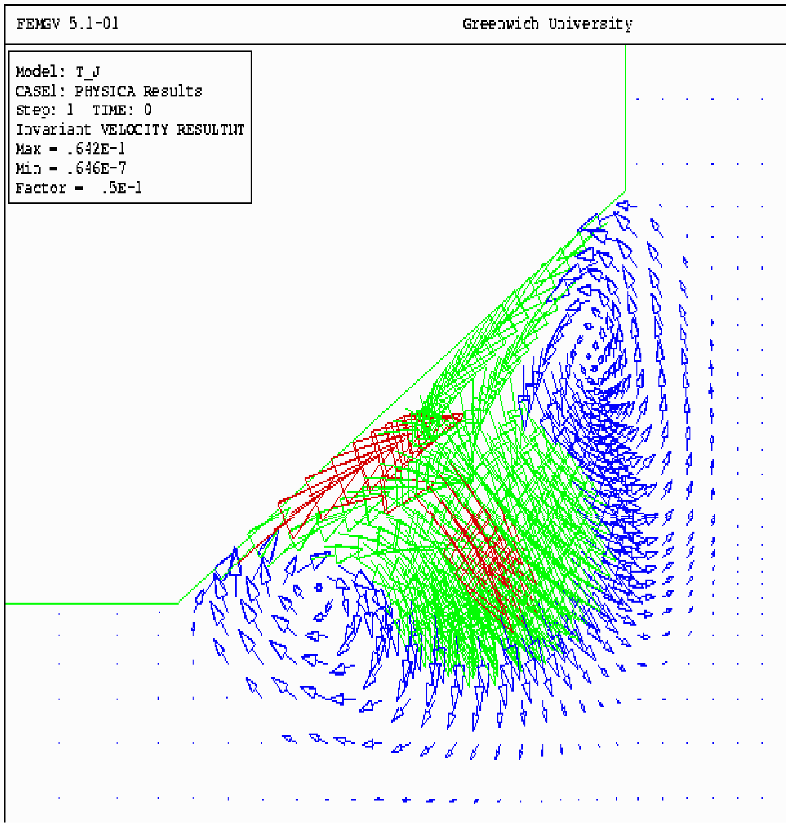
T-junction section,
highlighting HAZ region

Distortion of T-junction due to heat source

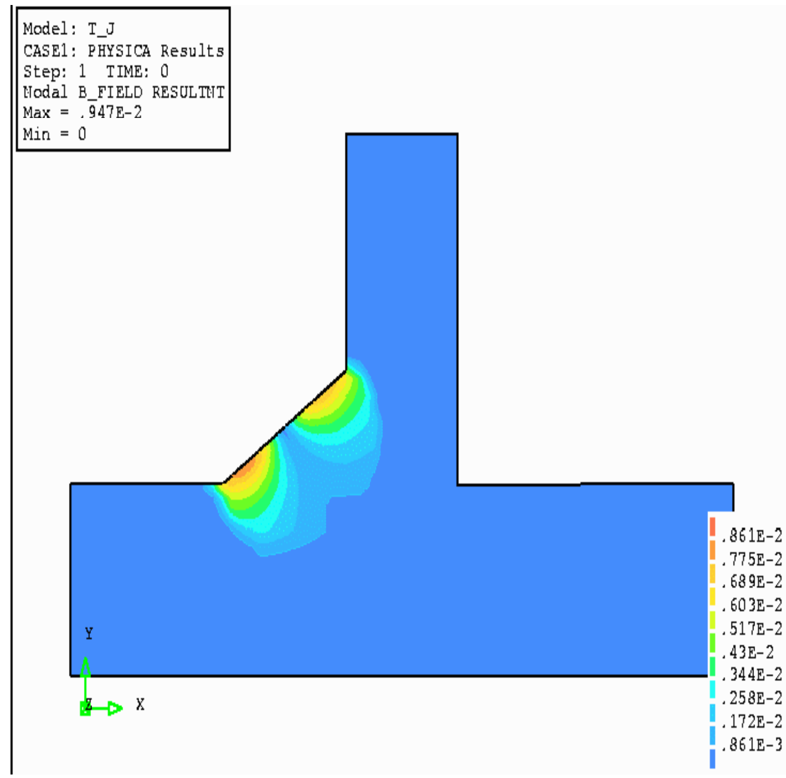


Heat source

Weld pool dynamics

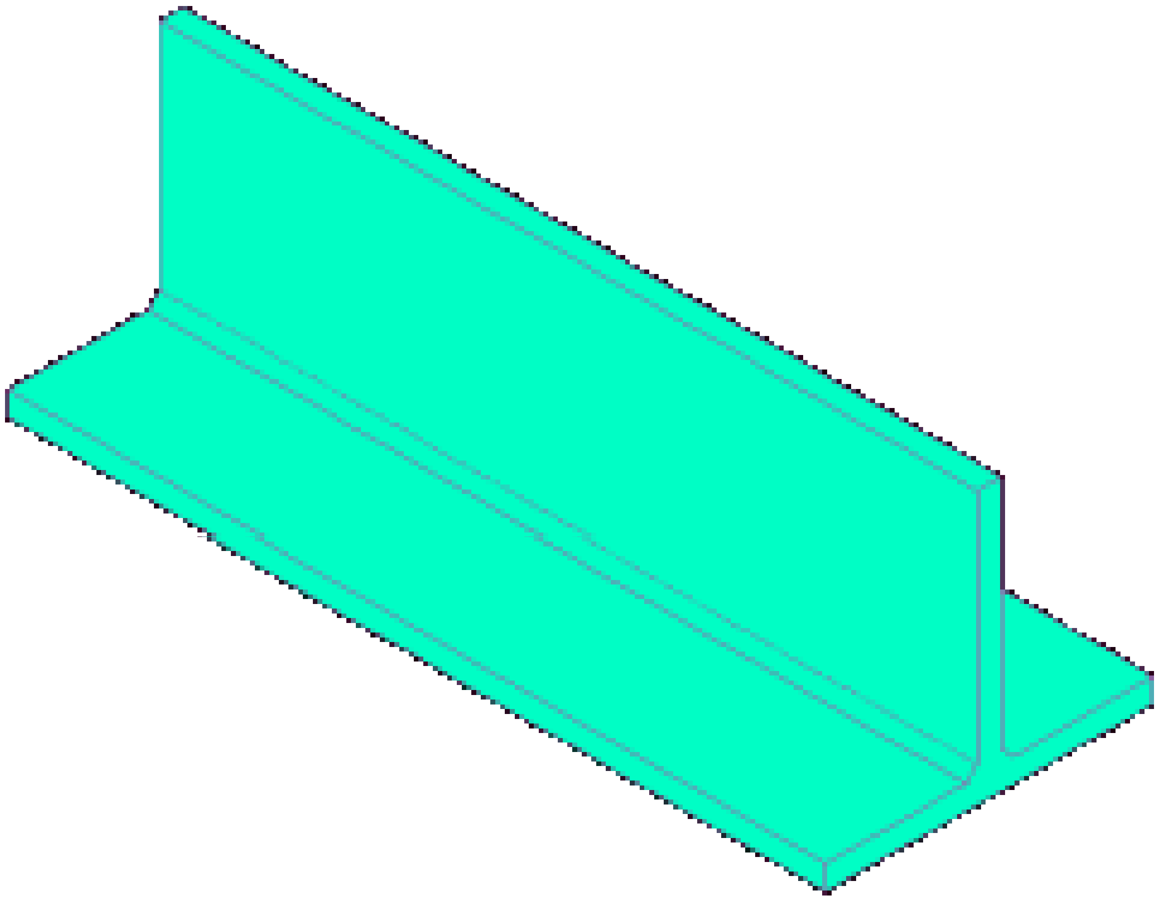


Velocity vectors in crossection



Lorentz force distribution in the weld-pool

Distortion of T-junction due to heat source



Welding – multi-physics BUT . .

- Welding involves:
  - free surface fluid flow
  - heat transfer and solidification/melting
  - electro-magnetic fields
  - non-linear stress

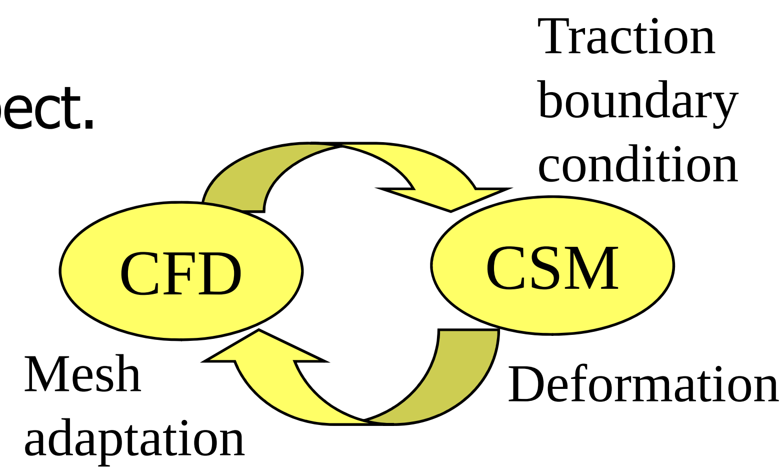
BUT . . no coupling back:

- from thermo-fluids to EM field
- from stress calculation to thermo-fluids

SO . . reasonably loosely coupled

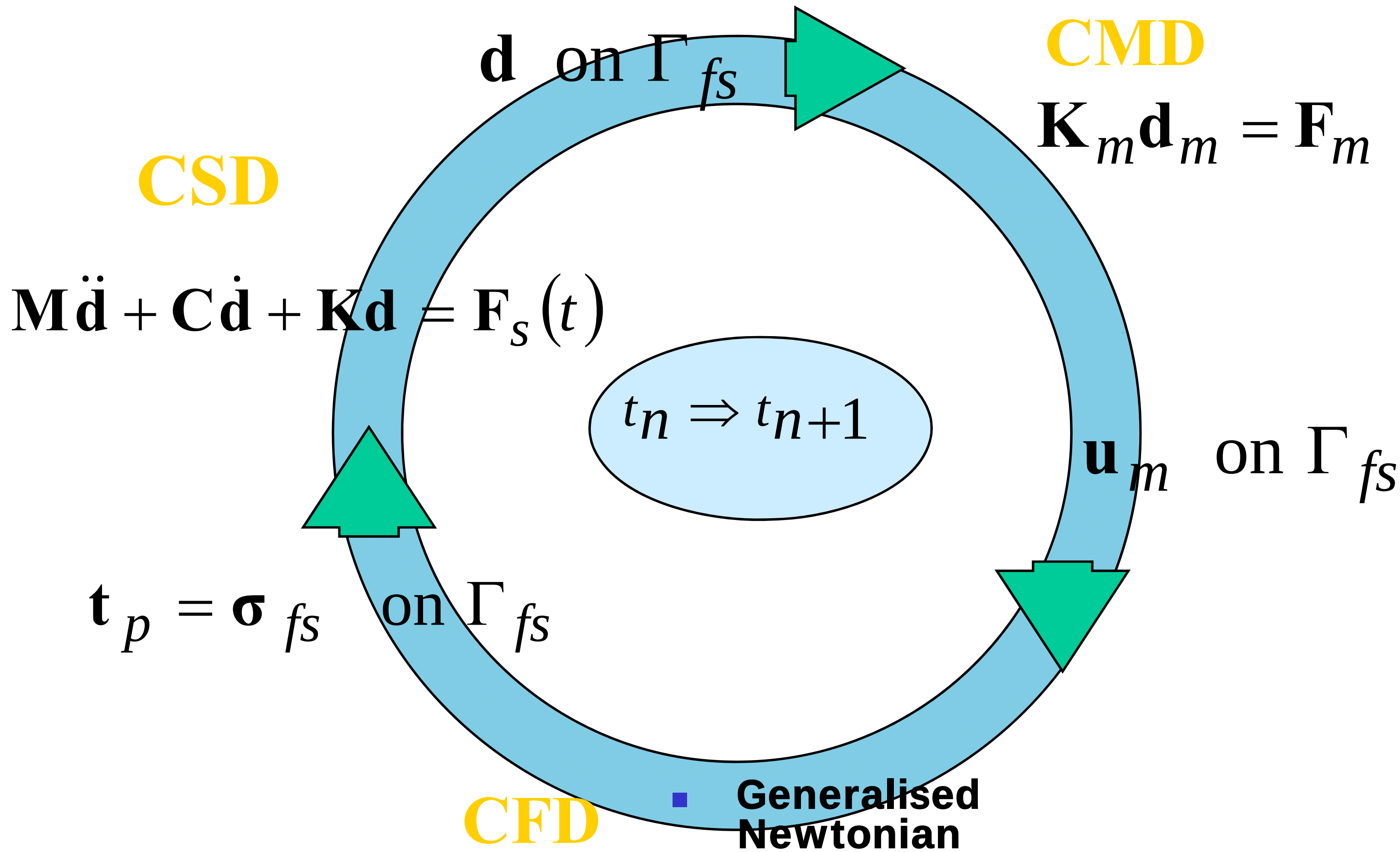
Generic Dynamic Fluid Structure Interaction

- Closely coupled multi-disciplinary problem
  - Time & space accurate
  - Very challenging in every respect.
  - Issue of GCL



  - Implementation of boundary conditions.
- Features of single software framework:
  - Consistency of mesh.
  - Single database & memory map.
  - Compatibility in the solution approaches FV-UM.

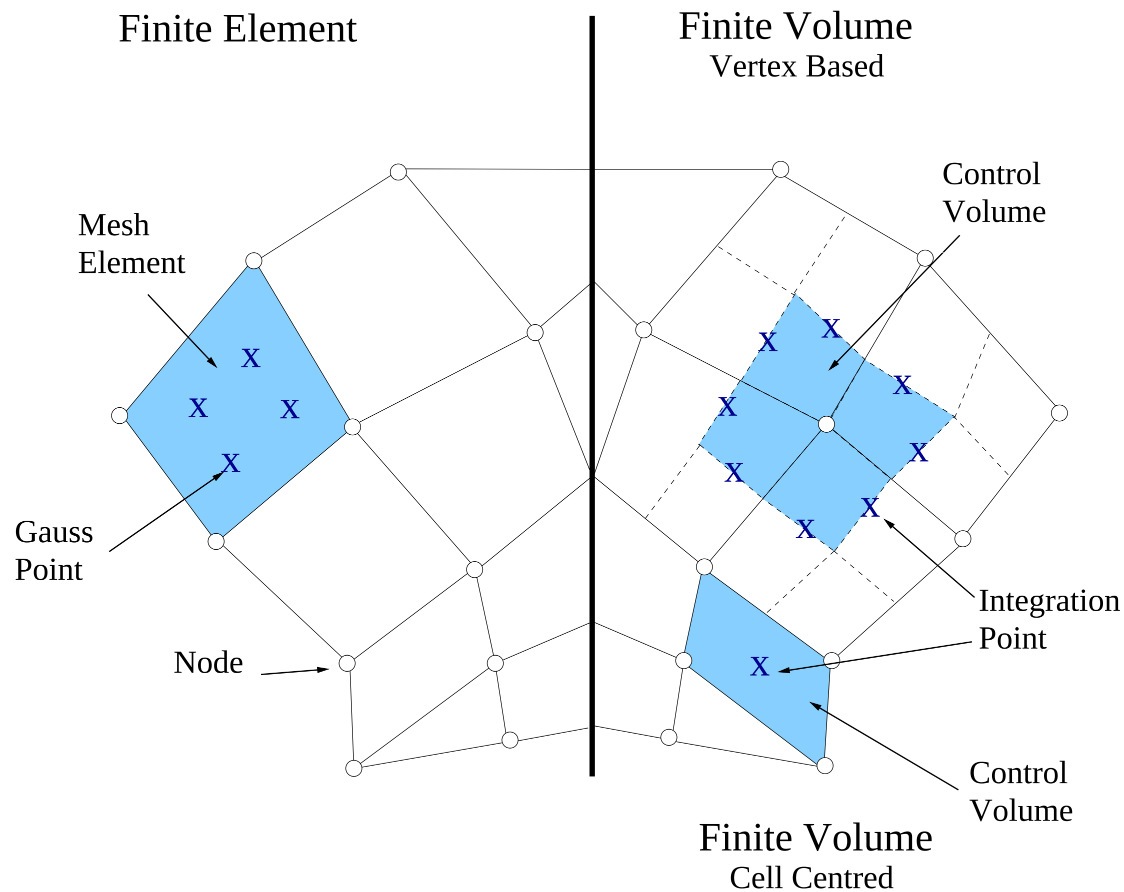
Three Phase Approach



- Generalised Newtonian
- Continuity

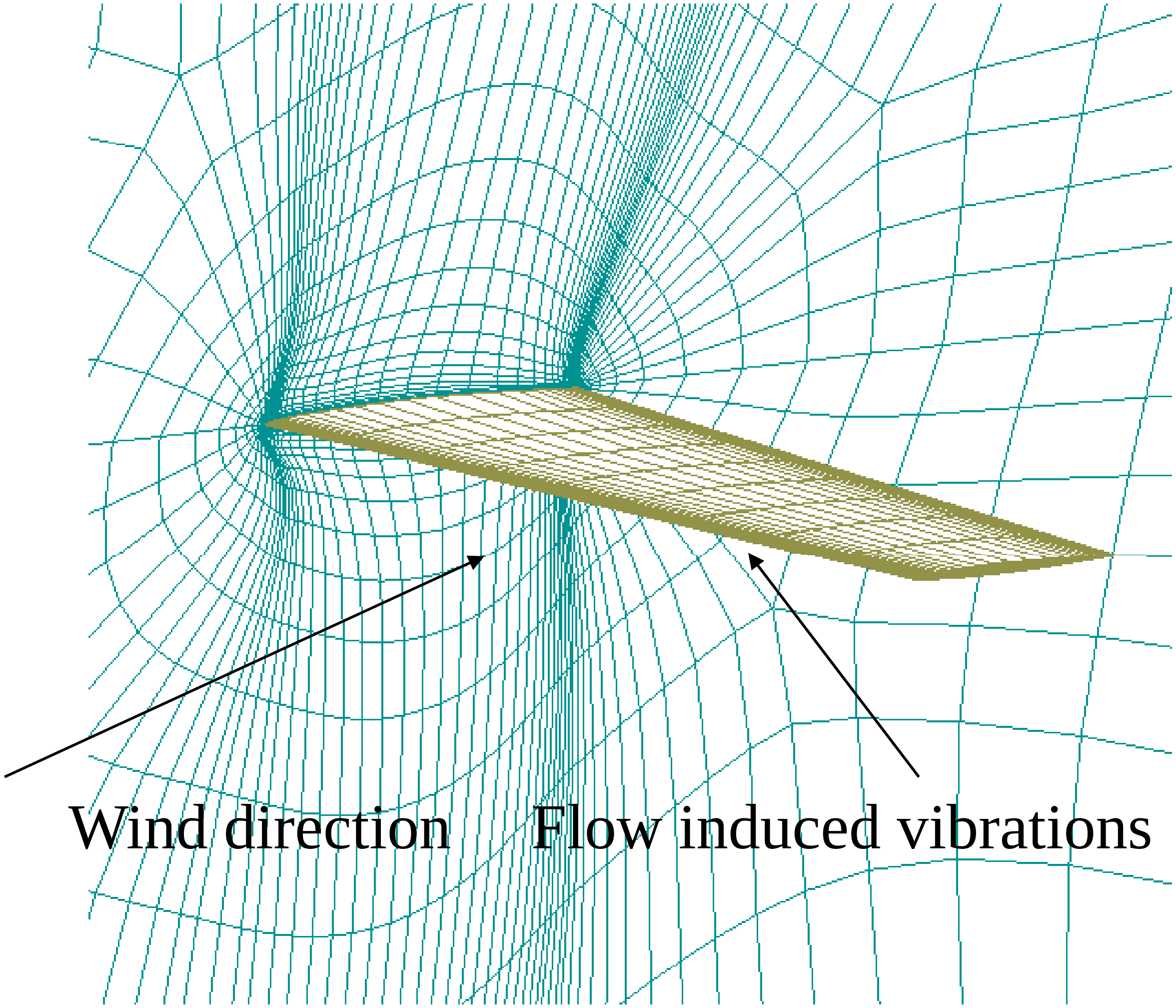
PHYSICA: Spatial Discretisation for closely coupled multi-physics

- Unstructured mesh
- CFD
  - Cell centred
  - Or mixed CC- VB
  - FV
- CSM
  - Vertex based
  - FV/FE

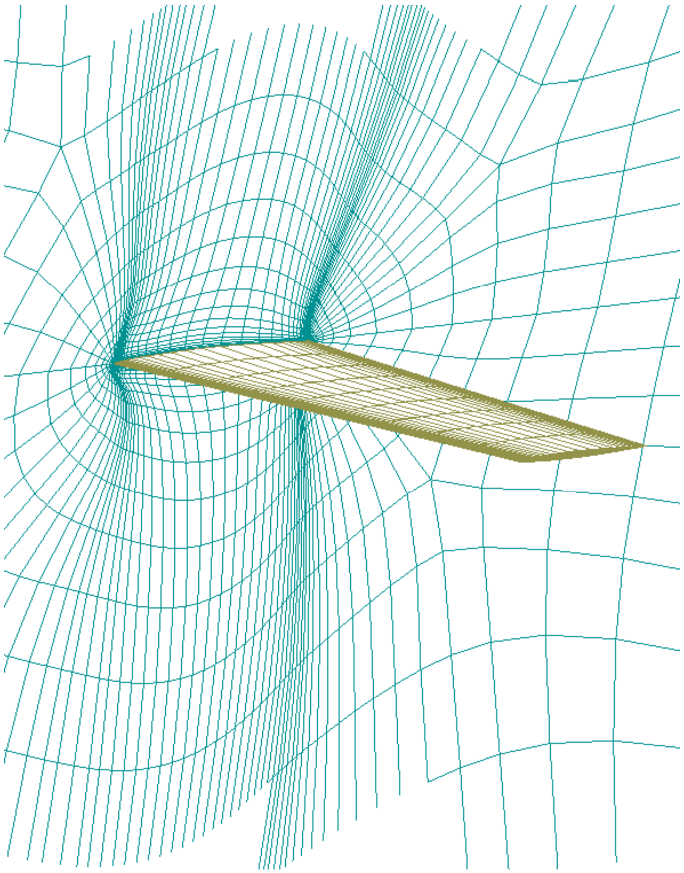


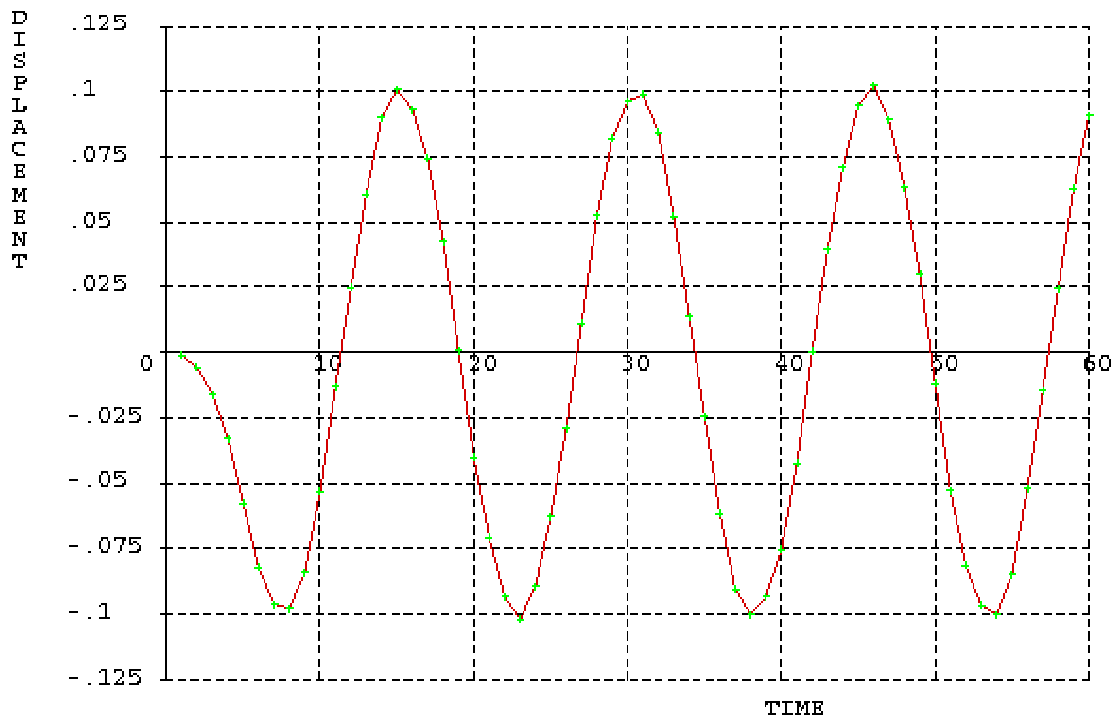
Dynamic fluid-structure interaction

- Targeted at problems involving flow induced vibrations
- Use dynamic structural equations and Navier-Stokes flow equations

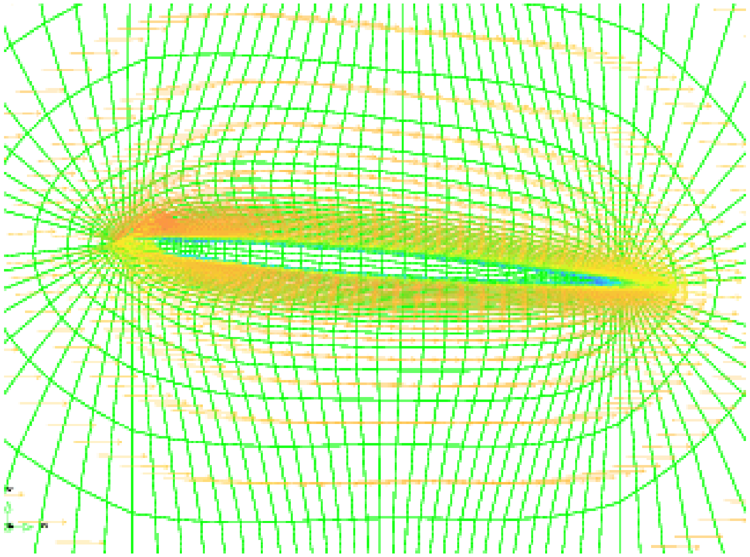


Dynamic response of structure without flow

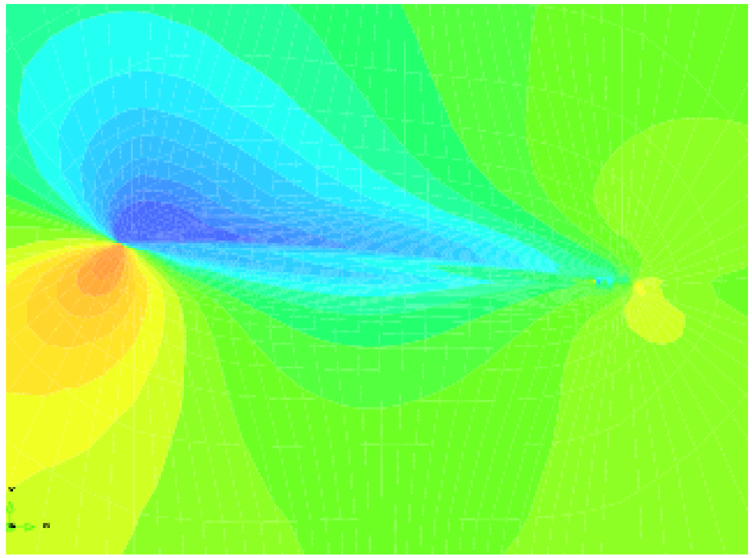




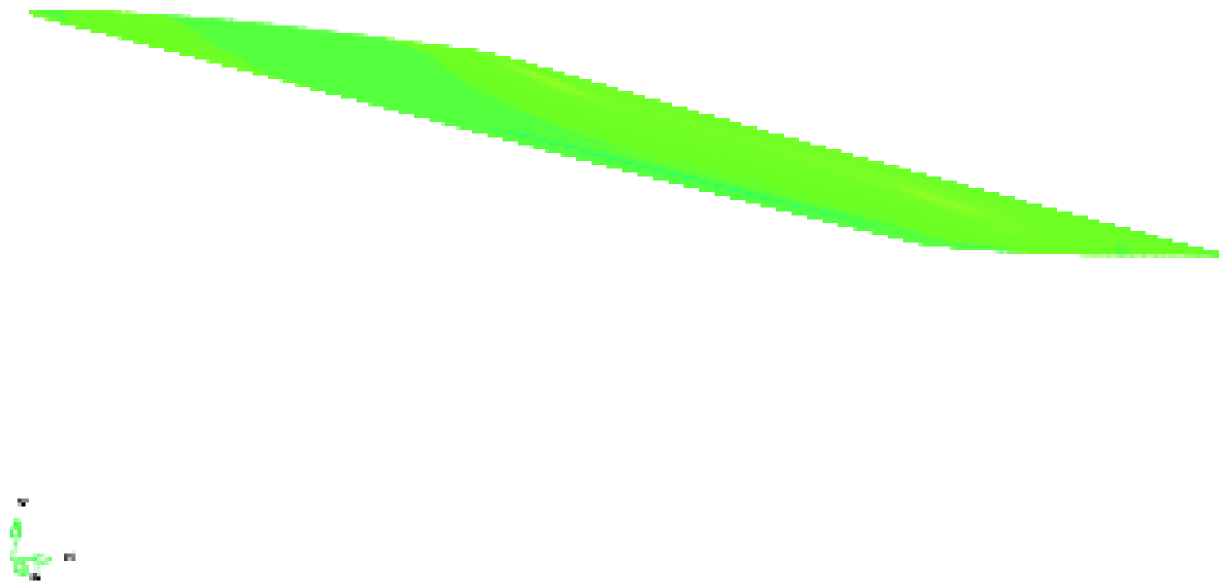
Fluid Velocity and Pressure Movies



At tip of wing



Shear Stress σ_{xy} Movie



Bio-medical multi-physics modelling: the heart!

- Heart – a multi-physics system, featuring interactions between:
  - electro-chemical system
  - fluid
  - structure

Geometry

- 2D model
- Right ventricle

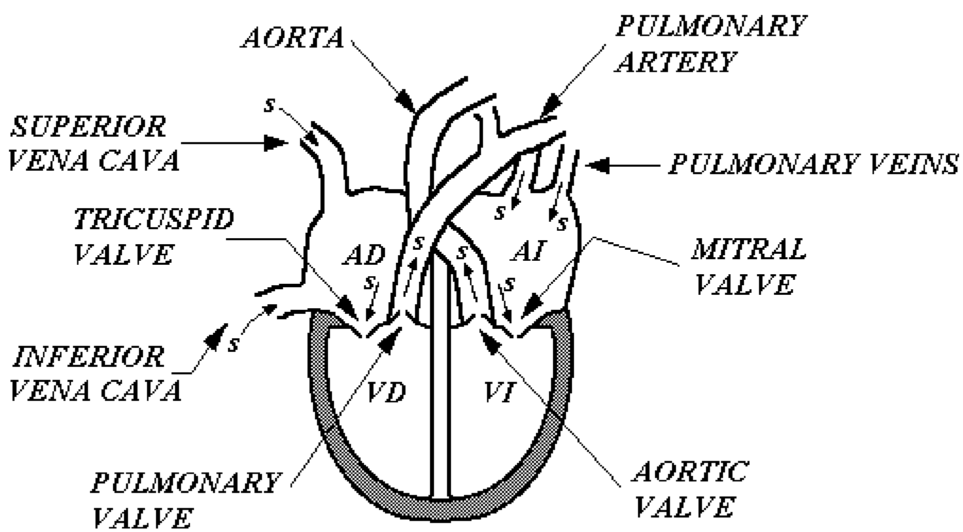
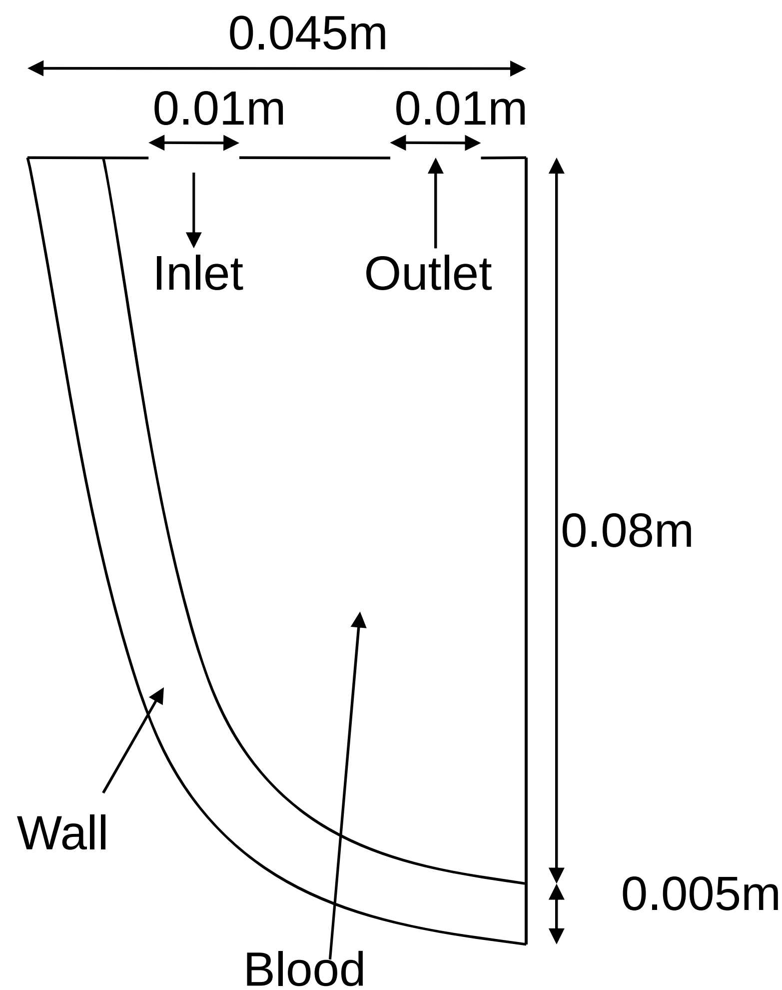
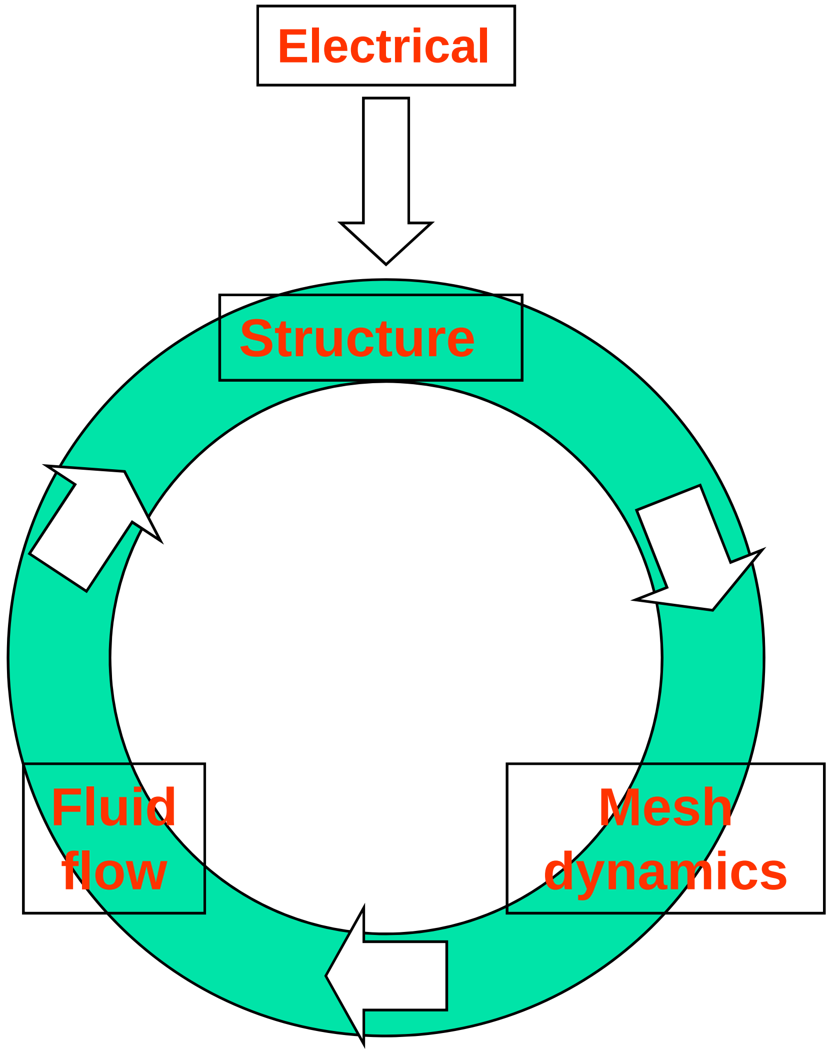


Image from www.heartvalves.8m.com



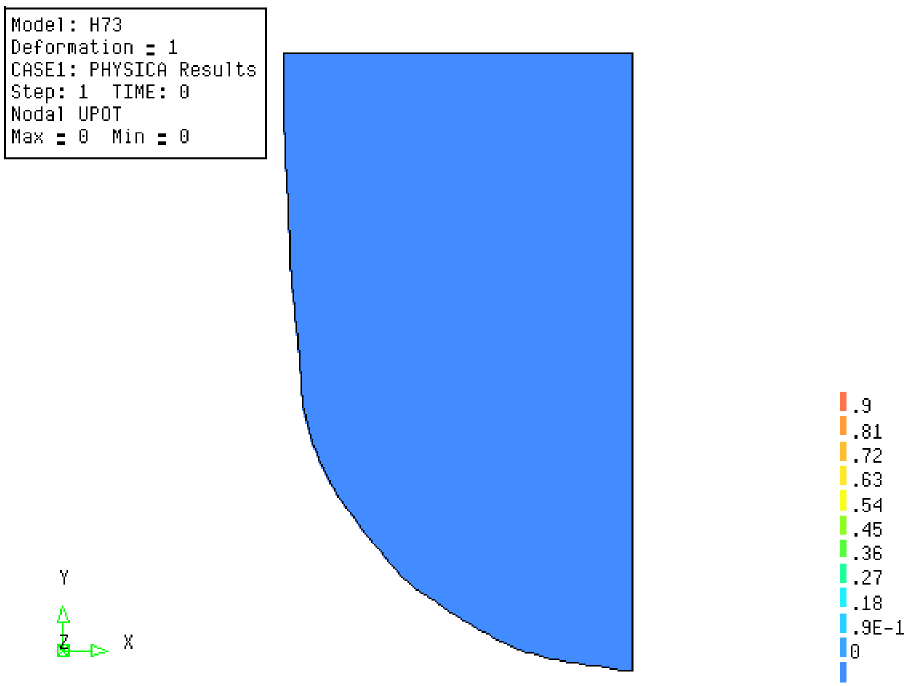
Electro-fluid-structure interaction

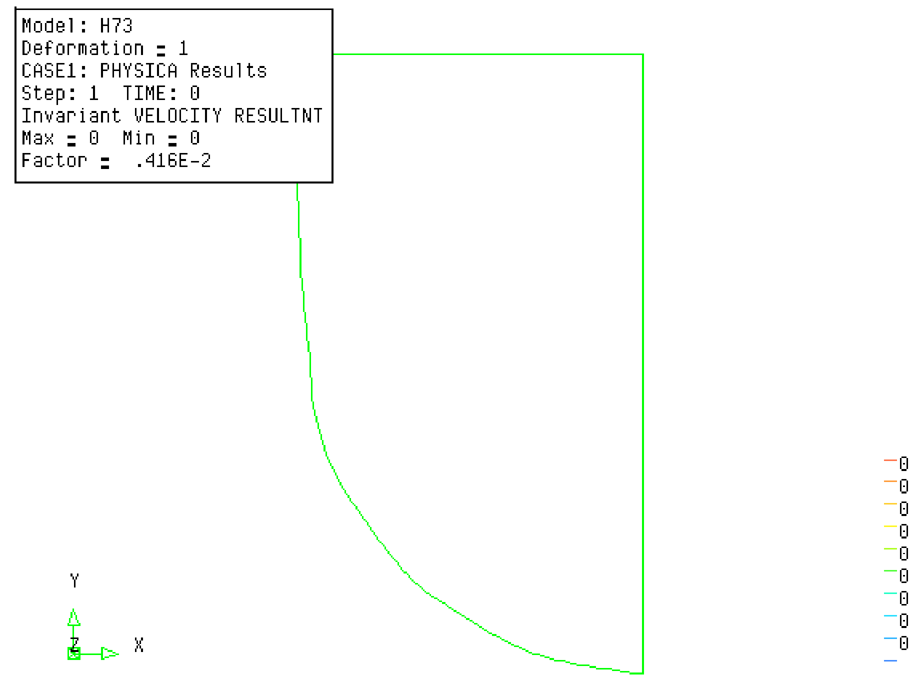


Coupling electrical field to structural mechanics

- Assumption made that small strain model can capture behaviour of heart wall
  - Dominant behaviour of wall is contraction/expansion
  - Shearing effects negligible
- Elastic model
- Change in potential results in a change in tension in the heart wall
- To model tension we introduce an electric strain into structural mechanics equations

Simulation results





- Δt=1E-4s
- 1 structure calc every 10 flow time-steps

- Calculation time ≈ 12 hours
- 6K element mesh
- 18 variables per node

Some health warnings on FSI

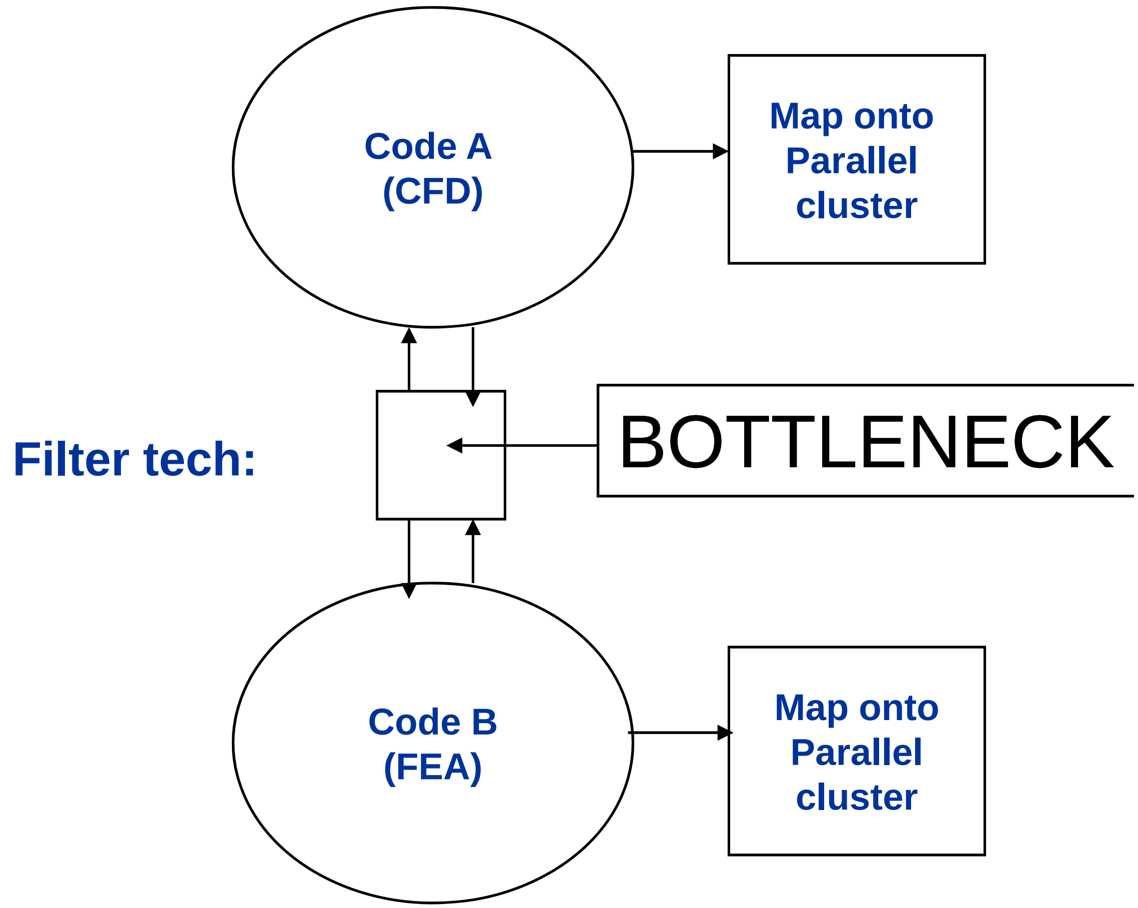
- Exchanging data between a CFD code & an FEA code does not amount to anything but loosely coupled FSI (e.g. welding)
- For anything other than coupled FSI:
  - Ask - at what level does the coupling occur?
  - Ask - is the procedure time and space accurate?
  - Ask - what tests have you done to ensure this is the case?
  - Ask – does your code include the GCL in its procedure?

Parallel Multi-Physics Modelling

NAFEMS World Congress
Vancouver, May 2007

Exploiting parallel cluster technology: the challenge

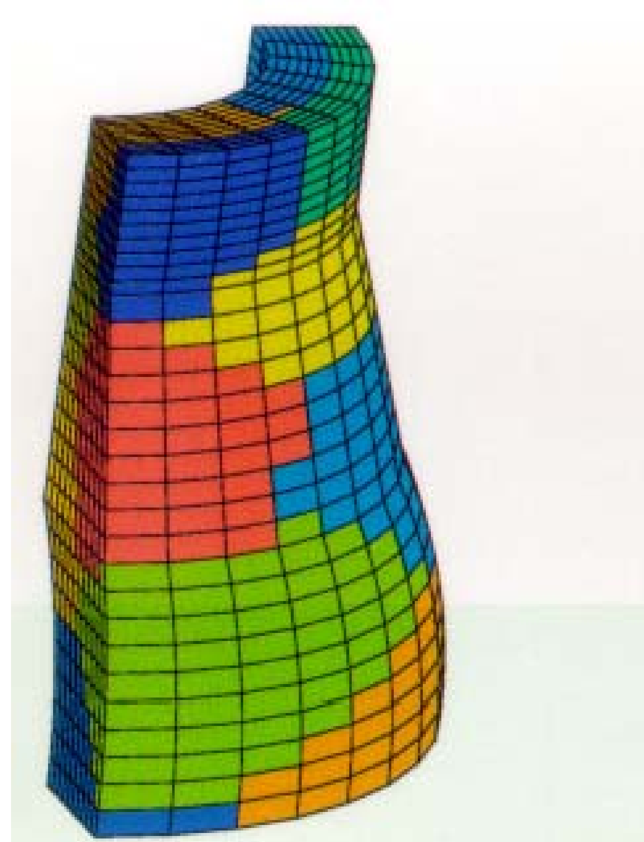
- MpCCI and other filter technologies
- Upside – enables interaction at the code d'base level
- Downside – all data exchange must go via filter and is a compute bottleneck wrt scalability on parallel clusters



Parallelisation approach uses mesh partitioning
SPMD strategy with non-uniform workload

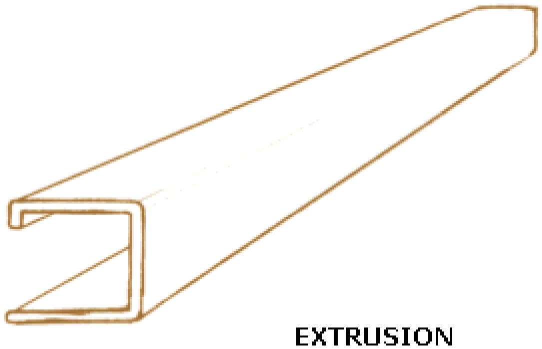
Partition of 3D unstructured mesh by JOSTLE assuming a homogeneous load balance across the mesh:

- **load balanced** (even no of cells per node)
- **minimises** sub-domain interface elements
- sub-domain connectivity **matches processor topology** of the parallel system



Metal Forming - Extrusion

- Involves large scale deformation of metal work-piece through interaction with one or more dies
- Multi-physics problem
  - Flow/deformation of work-piece
  - Heat transfer generated by internal friction
  - Stress/strain in die(s)



Mixed Eulerian-Lagrangian Approach

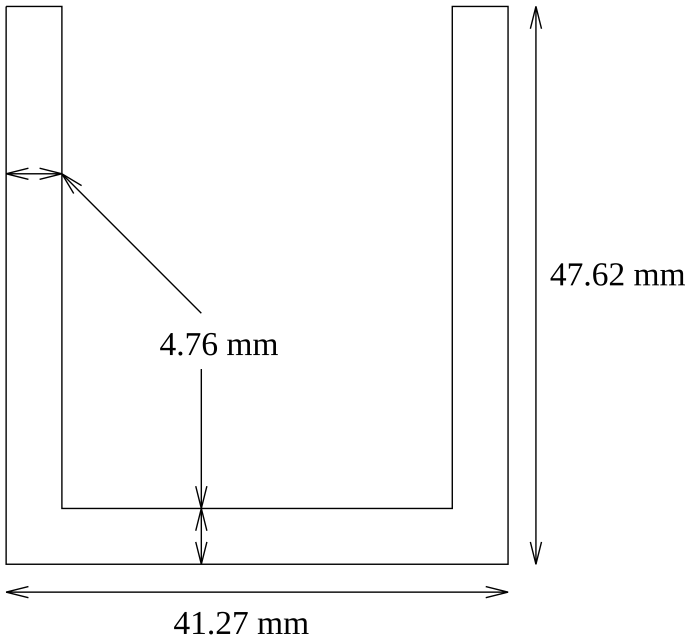
Workpiece

- Eulerian mesh
- Free-surface algorithm to track deformation
- Non-Newtonian material model
- Heat transfer plus energy generated by internal friction

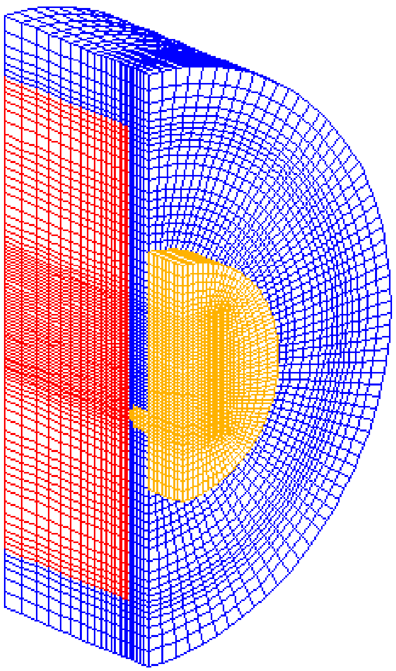
Die

- Lagrangian mesh
- Mechanical behaviour coupled with:
  - Thermal behaviour in workpiece
  - Fluid traction load from workpiece

Extrusion through U-shaped die



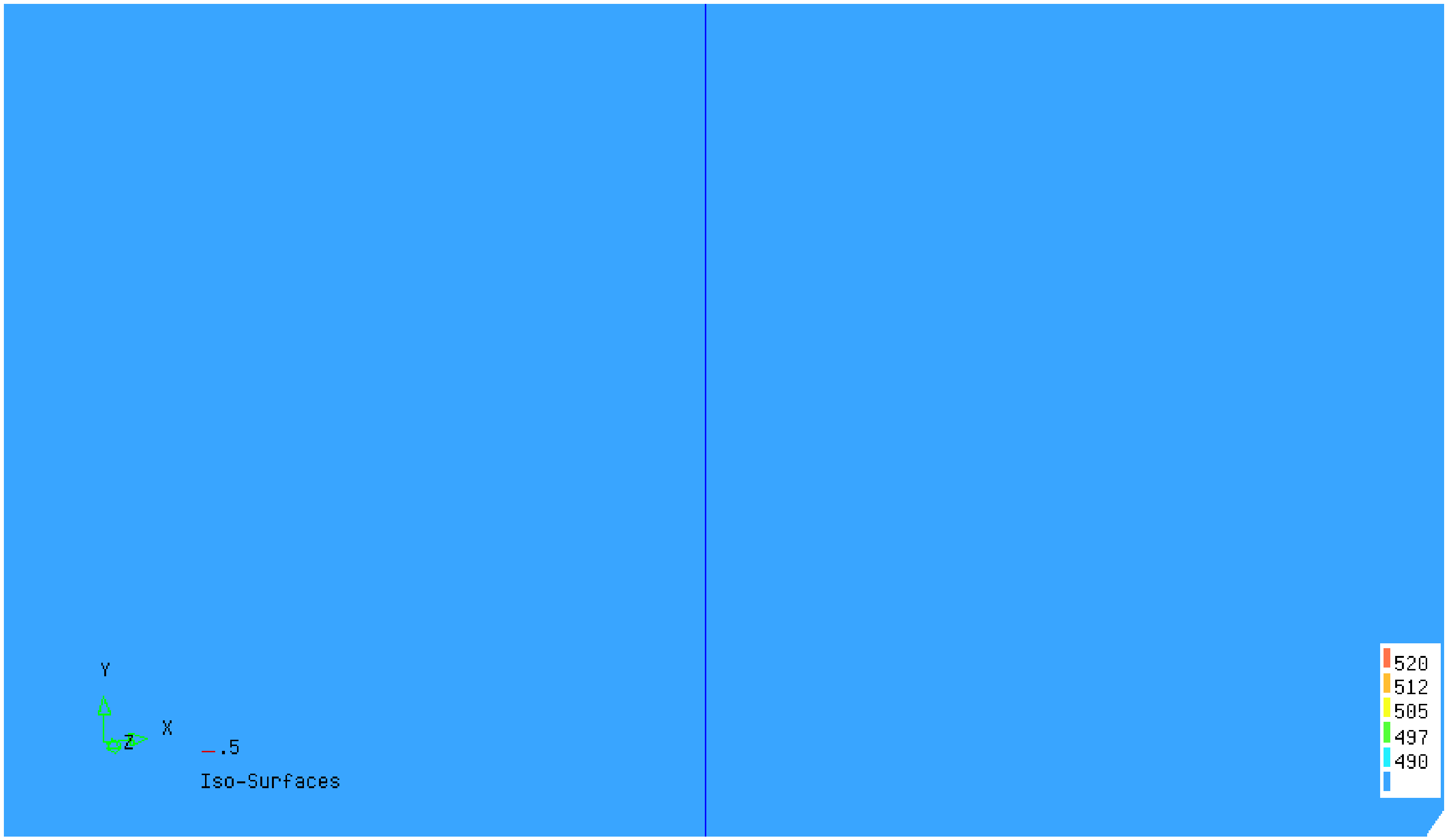
- **Initial diameter = 200mm**
- **Bearing length = 2.5mm**
- **Punch speed = 5.85E-3m/s**



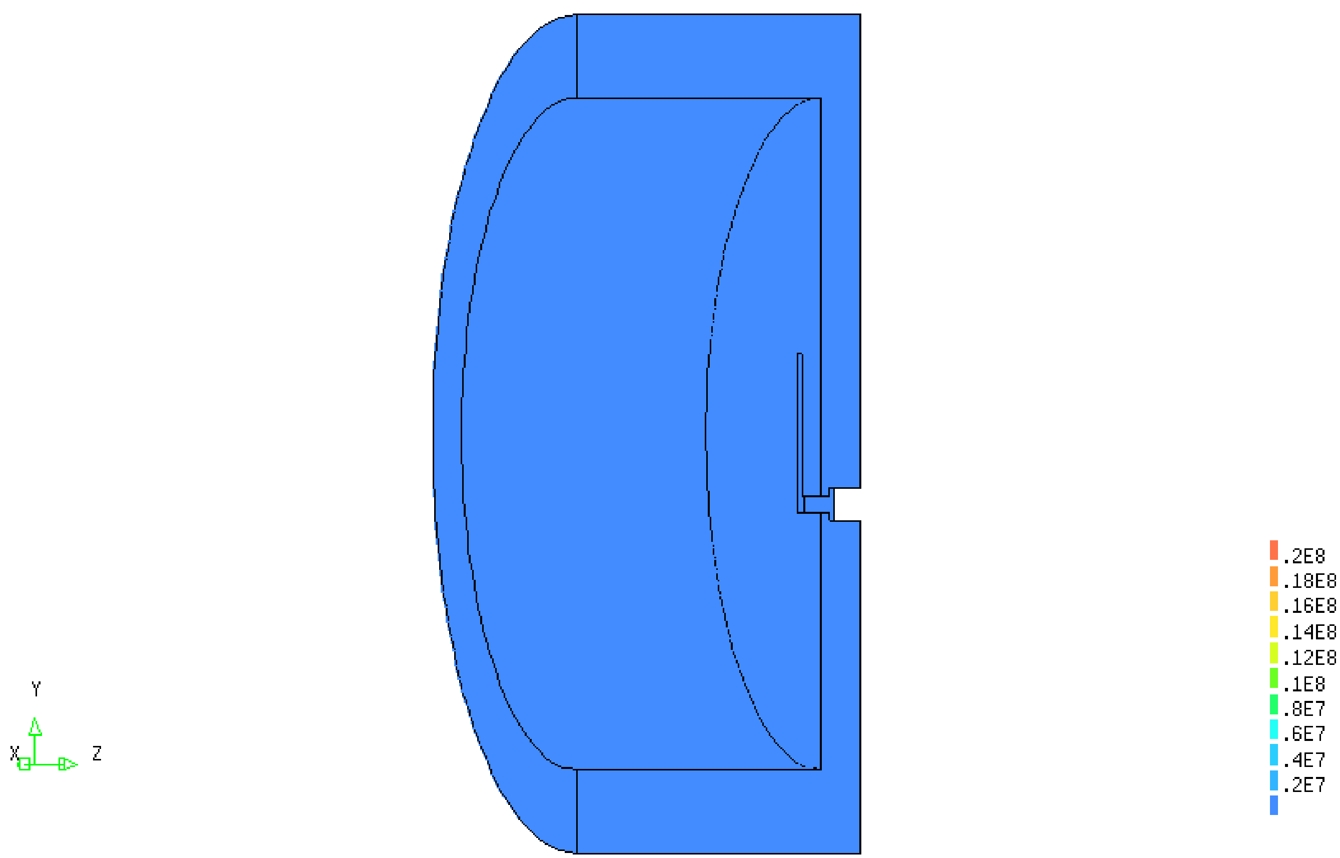
- 63220 elements
- 69507 nodes

- **Workpiece = 470°C**
- **Die = 450°C**
- **Air = 30°C**

Temperature contours in extruding work-piece

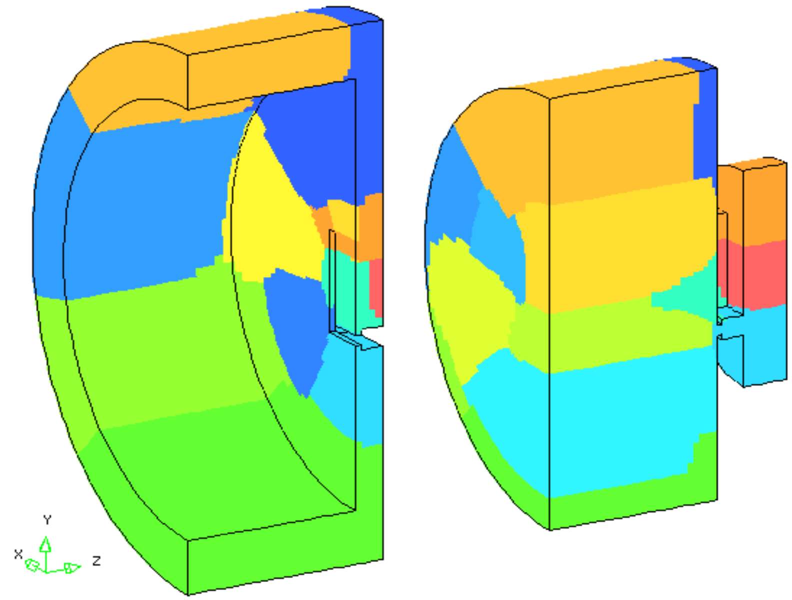


Effective stress contours and deformation of die



Parallel results

Processors	Run time (hours)	Speed-up
1	81.9	1
4	18.3	4.48
8	10.2	8.03
12	7.5	10.92
16	6.1	13.43



Single phase mesh partitions on 16 processors

- **Itanium IA 64 cluster running Linux OS**
- **Eight nodes, two 733MHz processors per node**
- **Each node with 2 Gb memory & 2Gb swap space**

Conclusion

- Multi-physics simulation is emerging in a commercially supported manner
- Most successful multi-physics is based upon loose or one-way coupling – even then, 'heroic computing'
- Close coupling in time and space another ball game - Key here are procedures for time & space accurate simulations; DFSI a key exemplar
- Multi-physics essentially compute intensive – leads to challenge of parallel scalability for multi-physics simulation tools
- Can do for bespoke single software solutions, but for multi-code components, not so clear!
- Challenges for the future – integrating components using essentially distinctive model paradigms & solver strategies