



MULTI-PHYSICS MODELLING AND SIMULATION: CHALLENGES AND OPPORTUNITIES

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Large number of real-world problems are multi-physics.

Electronic Packaging



Castings Components





- FEA started mid 60's with
 - NASTRAN, Abaqus, ANSYS, etc as major players
- CFD started 1980 with
 - FLUENT, CFX, PHOENICS and STAR-CD as major players
- MDA started mid 1990's
 - Coupling codes
 - MDICE, Spectrum, PHYSICA









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



🗑 Commercial Software – Multi-physics 🗶

- Number of products claiming to be multi-physics
- ANSYS/Multi-physics
 - http://www.ansys.com/
- PHYSICA
 - http://www.physica.co.uk/
- COMSOL
 - <u>http://www.comsol.com/</u>
- Algor
 - <u>http://www.algor.com/</u>
- DYNA
 - http://www.lsc.com
- ADINA
 - http://www.adina.com
- Flomerics
 - http://www.flomerics.com/







Classifying multi-physics



- What most vendors advertise is *multi-physics*
- What most vendors offer is *multi-disciplinary*
- Multi-disciplinary using data generated by one code as input into another – <u>loose or one way coupling</u> (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. thermomechanical)
- Closely coupled multi-physics time and space accurate exchange of data (e.g. dynamic fluid-structure interaction)

MDA vs. MULTI-PHYSICS

- Must distinguish between MDA and multi-physics:
 - one loosely coupled, other tightly coupled
 - one significant challenge, other major new technology development
- Multi-physics analysis always involves challenging flow analysis, so must be designed to compete well with leading edge CFD tools
- Limited CFD => limited multi-physics
- Limited parallel scalability => limited multi-physics











Multi-physics Modelling



Physics Requirements Fluid Flow **MULTI-PHYSICS** Heat transfer Solidification/phase change Stress **Electro-magnetics** Geometry **UNSTRUCTURED** Complex PARALLEL Large simulations **Key issue: CFD capability**







- Key players for thermo-fluid based models:
 - CFX
 - FLUENT
 - STAR-CD
- Key players for thermo-mechanical models:
 - ANSYS
 - ABAQUS
 - NASTRAN
- Key player for electro-magnetics:
 - OPERA & CONCERTO, Vector fields





- Most 'leading' CFD codes use FV methods on unstructured mesh
- All CSM codes based upon FE methods with a wide variety of element types
- CEM usually based on FE (and sometimes BE) methods
- Handling the physics interaction the challenge!





- Necessities:
 - phenomena specific solver software that can accept boundary data, volume source data and modifications to property data from other codes
 - good filters to exchange boundary and volume source data from one solver module to another
 - solver strategies which are compatible
- Practical demands:
 - Compatibility of the mesh structure
 - Very good filters for mapping numerical information from one solver to another
 - Avoid opening and closing files read numerical information directly from one solver by another; a common memory database is desirable
 - Parallel scalability is necessary for the large problems



Practicalities of multi-physics simulation



- Good numerical filters to map data from one solver into another
- Interpolation from one set of variables to another => compatibility of mesh
- 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?







- Coupled physics implies coupling of separate phenomena codes:
 - without opening/closing files
 - operate in a parallel context
- Emerged from an EU project public domain OPEN SOURCE tools
- www.scai.fraunhofer.de/mpcci.0.html
- Applications to fluid-structure interaction:
 - ABAQUS + FLUENT for DFSI
 - STAR-CD + NASTRAN for DFSI
- BUT exchanging data does NOT necessarily mean coupling of the physics that is time or space accurate







- Key route to closely coupled multi-disciplinary (multiphysics) 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



- COMSOL FEMLAB
 - Originally based on MATLAB as a suite of FE discretisation routines
- OEFELE Open Engineering
 - An FE based solver framework
- FOAM
 - solver framework for FE and FV discretisations

PHYSICA

- FV based tools for multi-physics



PHYSICA – Multi-physics Framework

- Work started in late 1980s at University of Greenwich
- Based upon FV methods on unstructured mesh (FV-UM)
- Conservative approach:

****FV-UM discretisation used for everything****

- Flow/ electro-magnetics/ heat transfer procedures from FV-SM -> FV-UM
- Solid mechanics developed from scratch
- Prototypes moved from:
 - a) 2 ->3D and
 - b) scalar -> parallel
- Key issue was to ensure FLOW worked well in all contexts
- Solidification processes a key target

Spatial Discretisation in PHYSICA









- Domain divided into a number of finite size control volumes (CV)
- Conservation equation integrated over each CV and time
- Approximations to each term yields a linear system in the unknown values of the variable \u00f6,

$$\frac{\partial(\rho\phi)}{\partial t} + \nabla \cdot (\rho\phi \mathbf{\underline{u}}) = \nabla \cdot (\Gamma\nabla\phi) + S_{\phi}$$







Cell-Centred (CC)



THERMO-FLUID MECHANICS



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





Mass and momentum

$$\frac{\partial}{\partial t} (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = \nabla \cdot (\mu \nabla \mathbf{u}) - \nabla p + \mathbf{S}$$
$$\frac{D(\ln \rho)}{Dt} + \nabla \cdot (\mathbf{u}) = 0$$

• Energy
$$\frac{\partial}{\partial t}(\rho h) + \nabla \cdot (\rho h \mathbf{u}) = \nabla \cdot (k \nabla T) + \mathbf{S}_{h}$$

Density

$$\rho = \rho(\phi_{metal}, \phi_{gas}) \text{ or } \rho = \rho_{flux}$$





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

















Release of energy due to phase change

$$S^{h} = -\frac{\partial}{\partial t} (\phi \rho_{m} f_{L} L) - \nabla \cdot (\phi \rho_{m} \mathbf{u} f_{L} L)$$

$$f_{L} = \begin{cases} 1 & T > T_{L}, the liquidus temp \\ \left(\frac{T - T_{s}}{T_{L} - T_{s}}\right) & T_{s} \leq T \leq T_{L}, in the mushy zone \\ 0 & T < T_{s}, the solidus temp \end{cases}$$

Darcy source for momentum equations





- CFD a mixed Lagrangian Eulerian calculation:
 - calculate the flow field using CFD procedure
 - use the flow field to influence the particle movement
- B/D/P equations (Argon bubbles in this case) are solved explicitly in Lagrangian framework.
- New position of each particle at given time-step computed from the particle equation of motion.
- Particle is subjected to a drag force C_d and buoyancy but no turbulence feedback.
- Drag force is an empirical function of the "slip" Reynolds number between particle and surrounding fluid.
- Account is taken of
 - the particles entering and leaving each computational cell
 - the time taken between entry and exit.
- Giving the instantaneous volume fraction of Argon in each cell, which is used to adjust the average density or other cell properties

Argon bubble injection: closely coupled L-E approach

C²EC





Solution domain







Solidification Strand

End





Clustering of argon bubbles



Solved using PHYSICA







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

Example: 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 $\frac{\partial \underline{B}}{\partial t} = \nabla \times (\underline{U} \times \underline{B}) + \eta \nabla^2 \underline{B}$ 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 $R_m (=LU/\eta) > 1$



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



B=0.4T

B=0T



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






Weld pool dynamics



Velocity vectors in crossection



4 F C

Lorentz force distribution in the weld-pool



Distortion of T-junction due to heat source







- 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

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





Generic Dynamic Fluid Structure Interaction

Closely coupled multi-disciplinary problem







Three Phase Approach







Spatial Discretisation for closely coupled multi-physics

Unstructured mesh

- CFD
 - Cell centred
 - Or mixed CC- VB
 - FV

CSM

- Vertex based
- FV/FE



C²EC





- Equilibrium Equation $\mathbf{L}^{\mathbf{t}} \boldsymbol{\sigma} + \mathbf{b} \rho \frac{d^2}{dt^2} (\mathbf{d}) = 0$
- Method of Weighted Residuals
 - Greens 1st theorem
 - where $\mathbf{d} \approx N_j \hat{d}_j$ evaluated at nodes

$$\int_{\Omega} \mathbf{W}_{i}^{T} \rho N_{j} \frac{d^{2} \hat{d}}{dt^{2}} d\Omega + \int_{\Omega} (\mathbf{L} \mathbf{W}_{i})^{T} \mathbf{D} \mathbf{L} N_{j} \hat{d} d\Omega - \oint_{\Gamma_{d}} \mathbf{W}_{i}^{T} \mathbf{T} \mathbf{D} \mathbf{L} N_{j} \hat{d} d\Gamma$$
$$= \int_{\Omega} \mathbf{W}_{i}^{T} \mathbf{b}_{0} d\Omega + \oint_{\Gamma_{t_{i}}} \mathbf{W}_{i}^{T} t_{p} d\Gamma + \int_{\Omega} (\mathbf{L} \mathbf{W}_{i})^{T} \sigma_{0} d\Omega - \oint_{\Gamma_{d_{i}}} \mathbf{W}_{i}^{T} \mathbf{T} \sigma_{0} d\Gamma$$





- Compact matrix form of equilibrium equation $\mathbf{M} \frac{d^2}{dt^2} (\hat{\mathbf{d}}) + \mathbf{C} \frac{d}{dt} (\hat{\mathbf{d}}) + \mathbf{K} \hat{\mathbf{d}} = \mathbf{f}$
 - where C is the damping matrix

$$\mathbf{M}_{ij} = \int_{\Omega_{i}} \mathbf{W}_{i}^{T} \rho N_{j} \, d\Omega$$
$$\mathbf{K}_{ij} = \int_{\Omega_{i}} (\mathbf{L}\mathbf{W}_{i})^{T} \mathbf{D}\mathbf{L}N_{j} \, d\Omega - \oint_{\Gamma_{d_{i}}} \mathbf{W}_{i}^{T} \mathbf{T}\mathbf{D}\mathbf{L}N_{j} \, d\Gamma$$
$$\mathbf{f}_{\mathbf{i}} = \int_{\Omega_{i}} \mathbf{W}^{T} \mathbf{b}_{0} \, d\Omega + \oint_{\Gamma_{d_{i}}} \mathbf{W}_{i}^{T} \mathbf{t}_{p} \, d\Gamma + \int_{\Omega_{i}} (\mathbf{L}\mathbf{W}_{i})^{T} \boldsymbol{\sigma}_{0} \, d\Omega - \oint_{\Gamma_{d_{i}}} \mathbf{W}_{i}^{T} \mathbf{T} \boldsymbol{\sigma}_{0} \, d\Gamma$$

• traction boundary condition on fluid – structure boundary $t_p = -p\delta_{ij} + \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{2}{3}\mu \nabla \cdot \mathbf{u}\delta_{ij}$ on Γ_s

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Essential difference between FE & FV Weighting Functions

• FE $\mathbf{W}_i = N_i$

direct association between N_i & *element*

 $FV \quad W_i = I$

within cv zero elsewhere

Mass matrix

FE

FV

 $\mathbf{M}_{ij} = \int_{\Omega_i} N_i^T \rho N_j d\Omega$ $\mathbf{M}_{ij} = \int_{\Omega_i} \rho N_j d\Omega$





Stiffness matrix $\mathbf{K}_{ij} = \int_{\Omega} \left(\mathbf{L} N_j \right)^T \mathbf{D} \mathbf{L} N_j d\Omega$ FE $\mathbf{K}_{ij} = -\oint_{\Gamma} \mathbf{T} \mathbf{D} \mathbf{L} N_j \, \mathrm{d} \Gamma$ **FV** Load vector • FE $\mathbf{f} = \int_{\Omega} N_i^T \mathbf{b}_0 d\Omega + \oint_{\Gamma} N_i^T t_p d\Gamma + \int_{\Omega} (\mathbf{L}N_i)^T \sigma_0 d\Omega$ • FV $\mathbf{f} = \int \mathbf{b}_0 d\Omega + \oint t_p d\Gamma - \oint \mathbf{T} \sigma_0 d\Gamma$ Γ_{t}





- **80x8x8**
- 5120 elements and 6561 nodes
- Analytic 2d solution Fenner v = 0



 3D cantilever, static results on Dec Alpha 466 MHz processor

	Iterations			Run times, second		
ν	FE JCG	FE-BICG	FV-BICG	FE JCG	FE-BICG	FV-BICG
0.3	539	540	544	48	95	98
0.2	483	483	483	44	85	88
0.0	438	438	437	38	78	80



Cantilever Dynamic Displacement







Fluid velocity & pressure fields





Re 4000





Cantilever interaction



Neutral z plane shear xy stress

Centre of cantilever length







Dynamic fluid-structure interaction



- Targeted at problems involving flow induced vibrations
- Use dynamic structural equations and Navier-Stokes flow equations
 - Objective: move to VB flow and FE based dynamics





Dynamic response of structure without flow







Fluid Velocity and Pressure Movies



At tip of wing





Shear Stress σ_{xy} Movie











Parallel Multi-Physics Modelling

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Multi-physics compute demands: secs per node(elt)/time step per problem class

- Unstructured Mesh analysis = 3* Structured mesh analysis
- Performance on a Compaq alpha 466Mhz
 - Heat Transfer (HT) + Solidification (Sol) = 2.10-3
 - Fluid Flow (FF) + HT + Sol = 6.10-3
 - HT + Sol + Stress = .09
 - -FF + HT + Sol + Stress = .14
- => a casting simulation with 100K nodes, and 100 time
 steps is 300+hrs!
- We need simulation times 100x faster

PARALLEL – WITH CHANGING PHYSICS







Single Program Multiple Data (SPMD)



- Program resident on each processor
- Mesh Partitioned across processors.
- Minimise communication times.



Simulations very Time Consuming – need Parallel capability





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



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Strategy needs to address all the above issues



- 2ndary partitions

- dynamic load balance

- Also, sub-domains may change as problem develops:
- Distinct physics uses

• Sub-domains have

specific physics so

partition must reflect this: - non-uniform load/node





Multi-physics Simulation parallel issues



Primary & secondary partitions



Primary & secondary (a) meshes

Good primary & poor Secondary partition (b)

Good primary & Secondary partitions (c) from JOSTLE





Parallel multi-physics: two level approach

Implement a generic parallel version of Multi-physics code/ MDA codes

- without regard to in-homogeneity of the computational work over the mesh(es) defining the analysis domain



 Dump the load balancing into the mesh (re)partitioning task -JOSTLE_DLB

Mesh Partition

PHYSICA

PDE Solver

 Process as straightforward as possible



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)









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 a conical die









- Coupled Thermo mechanical problem
 - Heat transfer significant factor in deformation process
- CFD
 - Non-Newtonian viscosity model Plastic Norton Hoff law
 - Heat Transfer Friction between die and workpiece.
 - Free Surface Van Leer method
- CSM
 - Static equilibrium equation linear elastic solid.
- Coupling at the workpiece/die boundary:
 - Die subject to fluid traction boundary condition.
 - Workpiece subject to a die velocity boundary condition.
 - Dynamic meshes GCL. Fluid velocity relative to mesh movement.



Governing Equations



- Free Surface
 - Scalar Equation Method ~ marker ϕ used to track free surface

$$\frac{\partial \phi}{\partial t} + \nabla (\boldsymbol{u} \cdot \boldsymbol{\phi}) = 0$$

Advection Scheme - Van-Leer

$$\phi_{face} = \phi_u + \frac{1}{2} \frac{\Delta \phi}{\Delta n} \left(d_{ud} - | \left(\boldsymbol{u} \cdot \boldsymbol{n} \right)_{face} | \Delta t \right)$$

- $\Delta\phi/\Delta n$ dependent on value of ϕ for upwind-upwind element
- Density Gradients GALA algorithm
- Coupled thermo-mechanical problem
 - Heat transfer significant factor in deformation process.
 - Energy entered into thermal equation as:

$$\frac{\partial}{\partial t} \left(\rho c_p T \right) + \nabla \cdot \left(\rho c_p \mathbf{u} T \right) = \nabla \cdot \left(k \nabla T \right) + \dot{r}$$

• Temperature development dependant on energy dissipation at rate:

$$\dot{r}_{ij} = \beta \sigma_{ij} \dot{\varepsilon}_{ij}$$

 $\boldsymbol{\beta}$ is proportion of plastic deformation energy dissipated as heat in solid material.



Extrusion through U-shaped die





• Air = $30^{\circ}C$



Temperature contours in extruding work-piece













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


Strengths and weaknesses:

- Cell centred methods:
 - memory efficient
 - fast

BUT

- accuracy fades rapidly as mesh quality degrades
- fails to converge with poor quality meshes
- correction terms help
 - slows convergence
 - stability

Cell-Centred (CC)







Strengths and weaknesses:

- Vertex centred methods:
 - heavy on memory
 - relatively compute intensive
 - good accuracy as mesh quality degrades
 - converges with almost any kind of mesh, no matter how poor its quality

Vertex-Based (VB)

CV Constructed around Mesh Vertex



Shape Function Approximations



Concept Of Approach for VB CFD





Increasingly skewed meshes for VB





Beltrami problem – 3D benchmark with analytical solution



Measured numerical errors for VB, CC and combinations

C²EC















Mesh element quality





Angle: Below 30° : Above 150°







- 118,314 Vertices, 101412 Elements
- Flow Variables (<u>u</u>, p) solved Vertex Based
- Turbulence k-e solved cell centred









Mach Number Turbulent Viscosity



a) C-mesh results

b) distorted C-mesh results





- Memory per Solution Point
 - Vertex-Based -> 373 Bytes
 - Cell-Centred -> 42 Bytes
- Seconds per Iteration / per Solution Point
 - Vertex-Based -> 3.3 x 10⁻⁵
 - Cell-Centred -> 7.0 x 10⁻⁶
- Number of Iterations
 - C-Mesh -> 254
 - Distorted Mesh -> 302



Example of VB-CC calculation: free surface capture



- SEA solves for the whole domain as a two component fluid and tracks the free surface development
- Uses D-A and van Leer schemes to sharpen surface capture
- Implemented using CC discretisation
- Procedure re-implemented using VB velocity components which are interpolated onto cell faces, and then hooked into conventional SEA







Key issue here is to test free surface procedure as the mesh quality is reduced

Mesh quality - non orthogonality ranges from 7 to 175 deg

CC has no chance of converging – question how does VB-CC method converge & how does accuracy degrade?



Simple test application: 2D collapsing column







Comparison with cartesian mesh









- Orthogonal Mesh
 - CC fast & efficient
 - No advantage in VB method
- Distorted (Non-orthogonal) Mesh
 - CC fails <u>OR</u> contains significant errors
 - Coupled VB-CC Method
 - Good global resolution of flow field
 - Enables solution of other transported quantities CC
 - Easily coupled with other well-established CC algorithms such as Scalar Equation Algorithm for free surface flow.



Challenging example



- Supplied by collaborator as an example of wheel
 - mixed elements
 - 91415 Elements
 - 55877 nodes
- No solution with the CC free surface SEA procedure















Problems with mesh quality







Boundary conditions & flows













The filling process









- Velocity is solved using a variant of SIMPLE with outer time step
- Free surface marker is tracked explicitly using smaller time steps
- Solved for 460 outer time steps to capture 8 seconds of real time
- Run on an Intel Pentium 4 2.53 Ghz processor with 83.62 MB memory
- Scalar run time 12 Hours
- Now implemented in parallel.







- Multi-physics simulation demanding of compatibility in specific phenomena solvers
- Key features of multi-physics simulation:
 - CFD capability
 - Fluid –Structure Interaction (FSI)
 - Parallel framework
- Our initial work very conservative in its initial FV methods on unstructured meshes for all phenomena
 - FV-CC for flow has limitations on mesh quality use VB-CC hybrid methods
 - FV for stress means reinvention of all FE stress solvers why?

Key challenges

- coupling complex flow physics into multi-physics solvers
- coping with extreme deformation with DFSI (e.g. parachute opening)
- coupling distinct physics (e.g. DEM with CFD)