Review and Advances of Coupling Methods for the ICFD solver in LS-Dyna



Coupled problems require the simultaneous solution of more than one physics module of LS-DYNA to obtain an accurate result.



Accurate CFD analysis will require structural coupling

The mechanical behavior of structural parts subject to heat and fluid pressure loads have been neglected.



Fluid Structure Interaction Roof vibration analysis



- CFD analysis of full vehicle.
- Couple parts of the structure to analysis the response in a realistic environment.



Fluid Structure Interaction

Three different options to solve the same problem:

- Solve Full Navier Stokes with FSI non linear coupling (using weak or strong coupling).
- Solve Potential flow with a non-linear step at the end.
- Solve the structural analysis alone using the output from Navier-Stokes (transient or steady state solver) and the *LOAD_SEGMENT automatically generated input deck. Use
 *ICFD_DATABASE_DRAG to write the files.

Fluid Structure Interaction. Results.



Velocity

Fluid Structure Interaction. Results.



Thermal Coupling



Thermal coupling

Options to solve the same problem:

- Solve Full Navier –Stokes with thermal non linear coupling (using monolithic or weak coupling). Shut off N.S after a certain steady state has been reached and continue with a pure thermal coupling analysis.
- Solve Navier Stokes using the steady state or potential flow solver and continue with conjugate heat transfer analysis once steady state has been reached.
- Solve the thermal analysis alone using the output from Navier-Stokes (transient or steady state solver) and the *BOUNDARY_CONVECTION_SET automatically generated input deck. Use ***ICFD_DATABASE_HTC** to write the files.

Conjugate Heat: Radiation

- Run steady state Navier-Stokes or Potential flow. Use
 ***ICFD_CONTROL_GENERAL** to set it up.
- Once steady state reached or Potential flow finishes the conjugate heat solver will use the steady velocity for the thermal analysis.





Conjugate Heat: Radiation. Results.



Conjugate Heat: Radiation. Results.



DEM Coupling



Recent developments introduced in R10 :

- Added Steady state solver. See ICFD_CONTROL_GENERAL and ICFD_CONTROL_STEADY.
- Added wave damping capabilities. See ICFD_DEFINE_WAVE_DAMPING
- Added Windkessel boundary conditions for blood flow. See ICFD_BOUNDARY_WINDKESSEL
- Option to output loads coming from the fluid and applied on the structure by using ICFD_DATABASE_DRAG keyword option. Similar feature for thermal and HTC and using ICFD_DATABASE_HTC
- Two way coupling with DEM particles
- Option to shut off Navier Stokes solve after a certain time for conjugate heat transfer analysis. See ICFD_CONTROL_TIME.

Currently working on :

- Periodic boundary conditions
- Sliding mesh capabilities
- Immersed FSI capabilities
- Monolithic FSI
- 1D parachute model.
- Boundary layer mesh improvements in complex geometry cases.

The EM solver. An overview of its uses and applications



Current main usage:

- The EM solver solves Eddy currents Using a coupled FEM-BEM method
- This implies that no air mesh
 is needed which allows complex shapes
 And strong deformations to occur

 The EM solver is therefore the perfect candidate to solve coupled mechanical thermal problems where strong deformations occur such as in Electromagnetic forming bending welding and so forth





Current main usage:

- More features have recently been introduced for such applications :
 - Axisymmetric solver (R10)
 - Conductivity function of material properties defined by the user with a DEFINE_FUNCTION
 - Option to define a circuit using a circuit equation and a DEFINE_FUNCTION to allow more complex types of circuits.
- Investigation is under way to add magnetic material capabilities through the introduction of an alternative monolithic solver.



Three new applications :

• Resistive Spot Welding (RSW) capabilities

- Extension of the resistive heating solver.
- Introduction of EM_ISOPOTENTIAL to define a potential difference between electrodes and EM_CONTACT_RESISTANCE to define a contact resistance
- Current capabilities are 3D, currently working on 2D solver.
- Battery short cut modelling
 - Extension of the resistive heating solver.
 - Introduction of circuit models to model ion transfers in batteries (See EM_RANDLES)
 - Extension of EM capabilities to Thick shells
- Cardiac solver for heart modelling
 - Extension of the resistive heating solver
 - Ten Tusscher & Panfilov cell models



Introduction - RSW



Electrodes on each sides of 2 sheets to be welded :

- Pressure
- Current flow => Joule heating => formation of a molten weld nugget

Coupled mechanical/EM/thermal simulations

RSW and contact resistance

In RSW, contact resistance plays a very important role in the heating of the nugget



New model in LS-DYNA for local contact resistance (in 3D) depending on local parameters, using *DEFINE_FUNCTION, e.g. Jonny-Kaars model :

$$r(T,P) = r_0 \left(\frac{p - p_k}{p_0 - p_k}\right)^{\varepsilon_p} \cdot \left(\frac{T - T_{\text{lim}} + (293, 15 \ K - T) \cdot 2^{-\frac{1}{\varepsilon_T}}}{293, 15 \ K - T_{\text{lim}}}\right)^{\varepsilon_T}$$

EM model for contact resistance (1)



EM model for contact resistance (2)

Contact resistance added in stiffness matrix



FEM solve:

 $(S_0 + D) * \phi = 0$ Where

- S₀ is the Laplacian operator (nodes x nodes)
- D has

•

- $1/r_s$ at (N_1, N_1) and (N_2, N_2)
- $-1/r_s$ at (N_1, N_2) and (N_2, N_1)
- 0 elsewhere

Row N_1 gives:

$$(S_0 * \phi)_{N1} + (D * \phi)_{N1} = 0 i_1 + 1/r_s (\phi_1 - \phi_2) = 0 (\phi_2 - \phi_1) = r_s i_1$$

And similar at row $\ensuremath{\mathsf{N}_2}$

On rows not connected to contact $S_0 * \phi = 0$ ensures the free divergence of the current in the plates (no charge accumulation)

23

Contact resistance depends on local parameters



EM cards to setup contact resistance



Typical RSW simulation



Current density

Temperature

Application

- The new LS-DYNA EM-Contact enables many approaches to cover the contact resistance for RSW
- The Jonny-Kaars-Model is an approach based on a resistance function of temperature and pressure where its parameter are fitted according experiments.

$$r(T,P) = r_0 \left(\frac{p - p_k}{p_0 - p_k}\right)^{\varepsilon_p} \cdot \left(\frac{T - T_{\lim} + (293,15 \quad K - T) \cdot 2^{-\frac{1}{\varepsilon_T}}}{293,15 \quad K - T_{\lim}}\right)^{\varepsilon_T}$$
pressure
temperature

Battery Abuse Simulations in LS-DYNA



Pierre L'Eplattenier, Sarah Bateau-Meyer, Iñaki Çaldichoury,

European LS-DYNA Conference, May 2017

Battery - Introduction

Vehicle







Battery – Distributed Randles circuit model



- Current collectors transport electrons to/from tabs; modeled by resistive elements
- Jelly roll (anode separator cathode) transports Li+ ions; modeled with Randle circuit



r₀: Ohmic & kinetic

 $r_{10} \mbox{ \& } c_{10} \mbox{:}$ Diffusion

u: Equilibrium voltage (OCV)

 r_m : Current collectors

Coupling between the solvers

Electrochemical

- Ordinary differential equations (Randles circuit model)
- Finite element analysis



Thermal

Finite element analysis; 3-D Heat diffusion with source terms



Structural

Finite element analysis; Nonlinear continuum mechanics



External short (1)

External short on a cell module



Sensors



Thermocouple locations



Cells and Bus Bar

Short circuit resistance applied between A and B creates current pathway

In collaboration with J. Marcicki et al Ford Research and Innovation Center, Dearborn, MI, USA

ONE FORD ONE TEAM • ONE PLAN • ONE GOAL

external short (1):

Model FExiped Wiser Nutrim Exptoin perature edele Valter On particular for each of the sent locations Experiment (Solid)



In collaboration with J. Marcicki et al Ford Research and Innovation Center, Dearborn, MI, USA



External short (2) Conducting cylinder falling on the tabs of a cell creates an external short



Randles circuits using Composite Tshells





Electrical connections using *EM_ISOPOTENTIAL and *EM_ISOPOTENTIAL_CONNECT

Composite Tshells: Keyword setup



Composite Tshells: Internal short (1)

Module of 10 adjacent cells crushed by a sphere

- Each cell is composed of
 - 228 *ELEMENT_TSHELL
 - 22 unit cells (89 layers)
 - 252 Randles circuit in each unit cell
- 55,440 Randles circuit total





time (s)

State Of Charge vs time

Composite Tshells: Internal short (2)

Same 10 cells module crushed by a cylinder



LS-PREPOST Battery Packaging



- Easy design of the layers of a single cell
- Addition of connecting tabs
- Multiplication of cells to create modules
- Electrical connections



€

Mat ID-

a

С



Positive Tab

Part ID:

Mat ID:

Thermal MatID: 0 . 4

Width00:

Length(Y):

Create Undo SaveProj Write K

0.03175

0.008



Battery – Plans for the future

- Collaborations with Ford Research and Innovation Center and Oak Ridge National Labs to improve:
 - Mechanical simulations of layered cells
 - Criteria for onset of internal short circuits
 - Setting of internal short resistance
- Development of more macroscopic models for modules and packs
- Addition of new features in LS-PREPOST battery packaging application

Electrophysiology modeling



Motivation

- Experimental studies involving the *in-vivo* human heart are possible and often available, but they are expensive and very limited.
- Well defined numerical modeling is emerging as a powerful tool that can help to interpret experimental data.
- Cardiac modeling is a complex problem. The maturity of the models of electrical propagation in the heart is still not comparable with the one achieved in other engineering fields mainly due to :
 - Non linear anisotropic inhomogenous material properties
 - Direct observation of electromechanical potential distribution is not trivial. Validation experimental results are difficult to obtain.
 - The problem not only involves multiphysics but is extremely multidisciplinary.

Electrophysiological models

The bidomain model : well-established description of the electrical activity of the myocardium on a macroscopic scale, taking into account the ionic current, the membrane potential and the extracellular potential.

The monodomain model : The monodomain model is a simplification of the bidomain equations. It assumes that conductivities are proportional in the intracellular and extracellular spaces

• GOAL

test the **ability** of LS-DYNA for cardiac tissue simulations

Benchmark:

Verification of cardiac tissue electrophysiology simulator using a N-version benchmark, Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences, vol 369, issue 1954, pp 4331-4351, November 2011



• BENCHMARK GOAL

Cuboid heart sample with stimulus on one corner. We observe the propagation of the potential inside the cell by determining the nodes' activation time.



• MODEL DEFINITION

Variable	Description
equations	monodomain
material	transversely isotropic
PDE solver	explicit
cell model	Ten Tusscher & Panfilov
variant	epicardium cell model
numerical integration scheme	Qu-Garfindel Operator Split
mesh type	hexahedral
solution method	finite element
basis function	linear Nedelec elements (FEMSTER)
pre-conditioners	none
matrix solver	hybrid-parallel, multifrontal, sparse direct solver (MF2)
system architecture	Serial or MPP

MODEL DEFINITION ۰

$$\begin{cases} \beta C_m \frac{\partial V}{\partial t} + \beta I_{ion}(u, V, t) - \nabla . (\sigma \nabla V) = I_{stim}(\vec{x}, t) & \text{monodomain equation} \\ \frac{\partial u}{\partial t} = f(u, V) & \text{cell model : ten Tusscher & Panfilov ionic equations} \end{cases}$$

V: membrane potential t:time σ : conductivity tensor C_m : membrane capacitance β : surface area to volume ration I_{stim} : stimulus current, applied at the position \vec{x} *I*_{ion} : single cell ionic current u : set of cell-level variables \rightarrow 19 for ten Tusscher model

explicit Qu-Garfindel Operator Split

$$V = V_t \qquad M.V_{t+1/2} = M.V_t - \frac{dt}{2\beta C_m}S.V_t$$
$$V = V_{t+1/2} \qquad V^*_{t+1/2} \begin{cases} C_m \dot{V} = I(u, V) \\ \frac{du}{dt} = f(u, V) \end{cases}$$

 $V = V_{t+1/2}^*$ $M.V_{t+1} = M.V_{t+1/2}^* - \frac{dt}{2\beta C_m}S.V_{t+1/2}^*$ Integrate diffusion PDE for half timestep

Projection onto the FEM basis functions $\beta C_m M. \frac{dV}{dt} + \beta I_{ion} - S. V = I_{stim}$ V , I_{stim} , $I_{ion} \rightarrow \text{nodal vectors}$ M: mass matrix $M(i,j) = \int_{\Omega} \Phi_i \Phi_j d\Omega$ S: stiffness matrix $S(i, j) = \int_{\Omega} \sigma \overrightarrow{\nabla \Phi_i} \cdot \overrightarrow{\nabla \Phi_j} d\Omega$

Integrate diffusion operator for half timestep

Integrate ionic operator for full timestep

9 SIMULATIONS

dx (mm)	number of elements	dt (ms)	number of time steps
0.5	3,360	0.05	1,600
0.2	52,500	0.01	8,000
0.1	420,000	0.005	16,000

• **RESULTS**

- 8 successful simulations - 1 failed simulation : dx = 0.1 mm with dt = 0.05 msCFL condition $dt \leq \frac{\beta C_m dx^2}{2\sigma_l \sigma_t} = 0.046 \text{ ms}$

The results are very similar to the benchmark paper ones



Activation time along P1-P8 for dt = 0.05 ms and dx = 0.5 mm, dx = 0.2 mm and dx = 0.1mm



ELECTRICAL POTENTIAL PROPAGATION



- Introduction of different solvers for the monodomain equations
- Introduction of bidomain model
- Presentation of the cards in LS-DYNA



• TO FACE THE CFL CONDITION



• TO GAIN TIME

Dave's Operator Split

explicit Dave's Operator Split

At even time step

numerical integration scheme

Integrate diffusion operator for one timestep

$$V = V_t \qquad M. V_{t+1} = M. V_t - \frac{dt}{2\beta C_m} S. V_t$$

Integrate ionic operator for full timestep

$$V = V_{t+1} \qquad V^{*}_{t+1} \begin{cases} C_{m} \dot{V} = I(u, V) \\ \frac{du}{dt} = f(u, V) \end{cases}$$

Set $V_{t+1} = V^{*}_{t+1}$

At odd time step

Integrate ionic operator for full timestep

$$V = V_{t+1} \qquad V^{*}_{t+1} \begin{cases} C_{m} \dot{V} = I(u, V) \\ \frac{du}{dt} = f(u, V) \end{cases}$$

Set $V_{t+1} = V^{*}_{t+1}$

Integrate diffusion operator for one timestep

$$V = V_t \qquad M.V_{t+1} = M.V_t - \frac{dt}{2\beta C_m} S.V_t$$

Machine time – simulation time = 80 ms (all the runs were done in serial)

Numerical integration scheme	dt1=0.05ms - dx1=0.5mm	dt1=0.05ms - dx3=0.1mm	dt3=0.005ms - dx3=0.1mm
explicit Qu-Garfindel Operator Split	1min14s	Х	33h15min30s
explicit Dave's Operator Split	59s	Х	24h49min3s
implicit Qu-Garfindel Operator Split	1min12s	3h23min58s	34h40min16s
implicit Dave's Operator Split	58s	2h32min30s	24h53min12s

TO INCREASE THE ACCURACY

equations	bidomain
PDE solver	implicit
numerical integration scheme	Spiteri-Ziaratgahi Operator Split

$$\begin{cases} \beta C_m \frac{\partial V}{\partial t} + \beta I_{ion}(u, V, t) - \nabla . (\sigma_i \nabla V) - \nabla . (\sigma_i \nabla u_e) = I_{stim}(\vec{x}, t) \\ \nabla . (\sigma_i \nabla V) + \nabla . ((\sigma_i + \sigma_e) \nabla u_e) = 0 \\ \frac{\partial u}{\partial t} = f(u, V) \end{cases}$$

bidomain equations

 u_e : extracellular potential

- σ_i : intracellular conductivity tensor
- σ_i : extracellular conductivity tensor

Projection onto the FEM basis functions $\beta C_m M \cdot \frac{dV}{dt} + \beta I_{ion} - S_i \cdot V - S_i \cdot U_e = I_{stim}$ $S_i \cdot V + S_{ie} \cdot U_e = 0$

implicit Spiteri-Ziaratgahi Operator Split

$$\begin{aligned} u_{t+1} &= u_t + dt \, f(u_t, V_t, t) \\ \begin{bmatrix} \frac{\beta C_m}{dt} M + S_i & S_i \\ S_i & S_{ie} \end{bmatrix} \cdot \begin{bmatrix} V_{t+1} \\ U_{e \, t+1} \end{bmatrix} = \begin{bmatrix} \frac{\beta C_m}{dt} M \cdot V_t - \beta M \cdot I_{ion}(u_{t+1}, V_t, t) \\ 0 \end{bmatrix} \end{aligned}$$

 $V, U_e, I_{stim}, I_{ion} \rightarrow \text{nodal vectors}$ 2 stiffness matrices $S_i(i, j) = \int_{\Omega} \sigma_i \overline{\nabla \Phi_i} \cdot \overline{\nabla \Phi_j} d\Omega$ $S_{ie}(i, j) = \int_{\Omega} (\sigma_i + \sigma_{ie}) \overline{\nabla \Phi_i} \cdot \overline{\nabla \Phi_j} d\Omega$

> solved using a PCG method, where the preconditioner is the diagonal line of the matrix, or with the hybrid-parallel, multifrontal, sparse direct solver, MF2

cell model

Purkinje





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Groups

Views

PtColor

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Appear

Annotat

Explod

Light & Reflect

Trace

SplitW

• INPUT DECK – MECHANIC (for now, i.e. for pure EP model without mechanical coupling)

*KEY	WORD							
*INC	LUDE							
mesh	.k							
\$ **	******	******	********	*******	******	******	******	******
\$ ME	CHANIC							
\$ **	******	******	*******	*******	******	******	******	******
*CON	TROL_TER	MINATION						
\$	1	2-	3	4	5	6-	7-	8
\$	endtim							
	80.							
*CON	TROL_TIM	IESTEP						
\$	1	2-	3	4	5	6-	7-	8
\$	dtinit					lctm		
	0.05					3		
*DEF	INE_CURV	Έ						
3								
0.,0	.05							
10.,	0.05							
*DAT	ABASE_BI	NARY_D3PL	.OT					
\$	1	2-	3	4	5	6-	7-	8
Ş	dt							
	0.2							
*PAR	T		-		_		_	
ş	1	2-	3	4	5	6-	/-	8
cell	ule							
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0.5.0		1						
*SEC	ITON_SOL	.1D	-		-		-	
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MAT		. 1						
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ς	motid	2-	3 F	4 pr	5	6-	/-	8
Ş	1 macia	0000 F7		pr 2				
	1	0720.31	200.0+09	.3				

• INPUT DECK – ELECTROMAGNETISM for MONODOMAIN



The conductivity is more important along the direction Y, which represents the fiber length.

INPUT DECK – ELECTROMAGNETISM for BIDOMAIN



emsol = $12 \rightarrow$



Definition of 2 conductivity tensors σ_i and σ_e

• INPUT DECK – CELL MODEL VARIABLES

*EM_EP_TENTUSSCHER

Variables linked to a material id

EM_I	EP_TENT	USSCHER						
ſ	matid 1	22-	3-	4-	5	6-	7-	8
COI	NSTS							
	1-	2-	3-	4-	5	6-	7-	8
C	onsts1	consts2	consts3	consts4	consts5	consts52	consts53	consts10
	R	Т	F	Cm	Vc	Vsr	Vss	p_KNa
83	14.472	3109	06485.3415	0.185	0.016404	0.0010940	.00005468	0.03
	1-	2-	3-	4-	5	6-	7-	8
COI	nsts11	consts12	consts13					
	K_o	Na_o	Ca_o					
	5.4	140.	2.					
	1-	2-	3-	4-	5	6-	7-	8
CO	nsts14	consts15	consts16	consts17	consts18	consts19	consts20	consts21
	g_K1	g_Kr	g_Ks	g_Na	g_bNa	g_CaL	g_bCa	g_to
	5.405	0.153	0.392	14.838	0.0002	0.0000398	0.000592	0.294
COI	nsts31	consts33						
	g_pCa	g_pK						
(9.1238	0.0146			-		_	
	1-	2-	3-	4-	5	6-	/-	8
COI	ists22	consts23	consts24	consts25	consts26	consts27	consts28	consts29
	P_Nak	K_MK	K_mNa	K_NACA	KSat	alpha	gamma	Km_Ca
	2.724	1.	40.	T000.	0.1	2.5	0.35	1.38
COI	1STS30	consts32						
1	07 E							
	07.5	0.0003	2-	4	5	6-	7_	0
	I-	consts35	consts36	consts37	consts38	consts39	consts/0	8
COI	151554 k11	k21	L0113 L330	kA	EC	may sr	min sr	
	0 15	0 045	0 06	0 005	1 5	2 5	1	
col	154541	consts44	consts42	consts45	consts43	2.5	1.	
001	V rel	V leak	V vfer	Vmax up	K un			
	0.102	0.00036	0.0038	0.006375	0.00025			
col	ists46	consts47	consts48	consts49	consts50	consts51		
	Buf c	K buf c	Buf sr	K buf sr	Buf ss	K buf ss		
	0.2	0.001	10.	0.3	0.4	0.00025		
IN	LT STAT	ES						
	1-	2-	3-	4-	5	6-	7-	8
S	tates1	states2	states3	states4	states11	states18	states19	
	V	K_i	Na_i	Ca_i	Ca_ss	Ca_sr	R'	
	-85.23	136.89	8.604	0.000126	0.00036	3.64	0.9073	
	1-	2-	3-	4-	5	6-	7-	8
s	tates5	states6	states7	states8	states9	states10	states12	states13
	xr1	xr2	XS	m	h	j	d	f
0	.00621	0.4712	0.0095	0.00172	0.7444	0.7045	3.373e-5	0.7888
sta	ates14	states15	states16	states17				
	f2	fCass	S	r				
(9.9755	0.9953	0.999998	2.42e-8				

• INPUT DECK - STIMULUS



ELECTRICAL POTENTIAL PROPAGATION - 2 STIMULUS



CONCLUSION

- Different EP models in LS-DYNA, for both monodomain and bidomain equations
- The ten-Tusscher cell model has been introduced
- They give good results on the first benchmark tests
- These models are available to the users through new cards
- More cell models will be added in the future
- What should be the priorities on pure EP?
 - Other cell models (Purkinje, ...)?
 - Introduce fractal Purkinje network ?
 - Try runs with many elements ?
 - Try runs with models closer to full heart with different cell models ?
- We are interested in the APD restitution results and whether more developments are needed to simulate tachycardia and fribrillation

