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MACALO

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Area: Nanoelectronics Technology (ICT-2009.3.1)

1st Intermediate report

Deliverable SIM-1

3D continuum transport equation solver treating heat, spin, and charge flow

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1 INTRODUCTION

As part of the overall MACALO's project In Silicio's main task is to develop a prototype 3D numerical solver able to accurately model coupled phenomena of heat, spin and charge transport in advanced magnetic nano-devices.

The present document materializes the delivery in time (at M12) of deliverable D1.1, a first working numerical implementation of the above introduced numerical solver.

2 CONSIDERED PHYSICAL TRANSPORT THEORIES

2.1 Coupled spin-charge transport

Before introducing the coupling with heat transport, let us recall first that coupled spin and charge transport phenomena in magnetic nano-structures can be theoretically formulated at different levels of transport theory, from quantum to classical; while retaining different level of time/space dependencies, from 3D time dependent equations to lumped element steady state circuit type theory.

It has been demonstrated over the last two decades that, among these various approaches, diffusive spin/charge transport theory, which was first rigorously derived from a two spin channels Boltzmann equation by Valet-Fert[2] , is among the best suited to aim at quantitative modeling of many devices of practical interests. This theory has been extended to non-collinear systems in the context of the so-called magnetic-electronic circuit theory[3], which have becomes increasingly of interest with the discovery and applications of spin-transfer torque[4] and spin pumping[5].

For coupled spin and charge transport, at the level of diffusive transport theory, the relevant physical degrees of freedom are the charge current $\vec{j}_c$ (a vector in 3D space), the spin current $\vec{\vec{j}}_s$ (in general a tensor quantity), the charge potential ϕ_c (a scalar), and the spin potential also often called the spin accumulation $\vec{\phi}_s$ (a vector in spin space).

So our starting points are the coupled spin-charge diffusive transport equations of the Valet-Fert theory, properly generalized to non collinear magnetic systems in a way consistent with the magneto-electronic circuit theory, and stated in three spatial dimensions. These equations can be split in two groups.

The first group of equations consists in linear response equations connecting currents with their conjugated potential gradients. Using the standard notation of the Valet-Fert theory, it reads:

$$\begin{pmatrix} \vec{j}_c \\ \vec{\vec{j}}_s \end{pmatrix} = -\frac{1}{\rho^*(1-\beta^2)} \begin{pmatrix} 1 & \beta/2 \\ \beta & 1/2 \end{pmatrix} \cdot \nabla \begin{pmatrix} \phi_c \\ \vec{\phi}_s \end{pmatrix} \tag{1.1}$$

Where the spin asymmetry coefficient β reduces of course to 0 in normal metals, and $\rho^*(1-\beta^2)$ is the experimentally measured bulk resistivity.

[2] T. Valet and A. Fert, Phys. Rev. B 48, 7099 (1993)
[3] A.Brataas, Y. Nazarov and G. Bauer, Phys. Rev. Lett. 84, 2481 (2000)
[4] J.C. Slonczewski, J. Magn. Magn. Mater. **159**, L1 (1996); L. Berger, Phys. Rev. B **54**, 9353 (1996)
[5] Y. Tserkovnyak, A. Brataas, and G.E.W. Bauer, Phys. Rev. Lett. 88, 117601 (2002)

This is supplemented by a second group of continuity equations for charge and spin, with the introduction of a finite spin diffusion length l_{sf} :

$$2\rho^* \nabla . \begin{pmatrix} \vec{j}_c \\ \vec{\vec{j}}_s \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & -1/{l_{sf}}^2 \end{pmatrix} \cdot \begin{pmatrix} \phi_c \\ \vec{\phi}_s \end{pmatrix} \tag{1.2}$$

It is important to recall that it has been demonstrated that in most situations of interest only the component of the spin current and spin accumulation *collinear to the local magnetization* survives in the bulk of ferro-magnets[6]. So, inside ferro-magnets the spin current can be most of the time safely assumed to reduce to an ordinary vector in 3D space $\vec{\vec{j}}_s = \vec{j}_s \otimes \vec{u}$ (with $\vec{u}$ a unit vector collinear with the local magnetization), while the spin accumulation reduces to a scalar $\vec{\phi}_s = \phi_s \vec{u}$. This approximation is relaxed in the context of the 3D CRMT type theory which will be further developed by the CEA partner as part of WP1, and a related numerical solver will be delivered at month 18 as deliverable D1.2 (SIM-2).

One has also to note that we consider here only time independent (steady state) equations. The rationale for this is the significant time scale separation between electron diffusion time scale across typical nano-devices of interest (of the order of 10^{-13}s), and typical time scale for magnetization precession and/or for applied external excitations for the same devices (typically of the order of 10^{-10}s). The same will apply for heat diffusion equation later on.

These volume equations have to be supplemented by proper interface boundary conditions at any F/N interface. As previously mentioned, the appropriate conditions have been derived from quantum transport theory in the general case of non-collinear magnetic structures in the context of the magneto-electronic circuit theory (we rewrite them here with notations consistent with the Valet-Fert theory):

$$\vec{n}_{(F)} \cdot \vec{\vec{j}}_s^{\,(F)} + \left[\vec{u} \cdot \vec{\vec{j}}_s^{\,(N)} \right] \cdot \vec{n}_{(N)} = 0 \tag{1.3}$$

$$\vec{n}_{(F)} \cdot \vec{j}_c = -\frac{\phi_c^{(N)} - \phi_c^{(F)}}{r_b^*(1-\gamma^2)} - \gamma \, \frac{\vec{u} \cdot \vec{\phi}_s^{(N)} - \phi_s^{(F)}}{2\, r_b^*(1-\gamma^2)} \tag{1.4}$$

$$\begin{aligned} \vec{n}_{(N)} \cdot \vec{\vec{j}}_s^{(N)} = & \left\{ \gamma \, \frac{\phi_c^{(N)} - \phi_c^{(F)}}{r_b^*(1-\gamma^2)} + \frac{\vec{u} \cdot \vec{\phi}_s^{(N)} - \phi_s^{(F)}}{2\, r_b^*(1-\gamma^2)} \right\} \vec{u} \\ & + g_{\uparrow\downarrow} \left\{ \vec{\phi}_s^{(N)} - \left[\vec{u} \cdot \vec{\phi}_s^{(N)} \right] \vec{u} \right\} \end{aligned} \tag{1.5}$$

Where $\vec{n}_{(\Omega)}$ is a unit vector at the interface which is the local normal vector outgoing from region (Ω). In analogy with the bulk case one introduces an interfacial resistance spin asymmetry coefficient γ ; with $r_b^*(1-\gamma^2)$ the experimentally measured interfacial resistance (minus the so called spin coupled resistance). The non collinear case introduces one

[6] M.D. Stiles and A. Zangwill, Phys. Rev. B 66, 014407 (2002)

additional (interface) material parameter, the spin mixing conductance $g_{\uparrow,\downarrow}$ (here we neglect its imaginary part, which is an appropriate approximation for metal-metal interfaces).

We have also left out of the right hand side of equation (1.5) the spin current source term originating from spin pumping effects, which will have to be considered at a later stage for adequate coupling with magnetization dynamics.

In general appropriate external boundary conditions at contacts which can be of either Dirichlet (fixed potential) or Neumann (forced current) types have also to be specified in order to generate a well posited boundary value problem.

2.2 Thermoelectric system

At the same level of diffusive transport theory, coupling between thermal and charge transport, leading to so called thermoelectric phenomena, is of course a textbook classic. Introducing a local temperature T and heat current $\vec{j}_Q$, the thermoelectric linear response equations read:

$$\begin{pmatrix} \vec{j}_c \\ \vec{j}_Q \end{pmatrix} = -\frac{1}{\rho}\begin{pmatrix} 1 & S \\ \Pi & \rho\kappa \end{pmatrix}\cdot\nabla\begin{pmatrix} \phi_c \\ T \end{pmatrix} \tag{1.6}$$

With κ the thermal conductivity, S the Seebeck coefficient and Π the Peltier coefficient; while the continuity equation for heat flow is:

$$\nabla.\vec{j}_Q = -\vec{j}_c.\nabla\phi_c \tag{1.7}$$

Where we have assumed in the above equation that the only dissipated power density source term is from Joule effect heating.

Again these volume equations have to be supplemented by proper interface boundary conditions, with the possible introduction of interfacial thermal resistances, interfacial Seebeck/Peltier coefficients, and associated interface dissipation.

Appropriate external boundary conditions which can be of either Dirichlet (fixed temperature) or Neumann (forced heat flow) types have also to be considered.

2.3 General spin caloritronic system

As maybe first envisioned by Johnson and R.H. Silsbee[7], while considering a device structure that would be called nowadays a lateral spin valve structure, and much later on investigated experimentally in magnetic multilayers and further developed theoretically by the Lausanne's group[8], new phenomena arises when one considers simultaneous transport of spin, charge and heat in metallic hetero-structures, leading to the emergence of what we call now spin caloritronics[9]. When considering all things together, the complete set of linear response equations in the bulk reads now:

[7] M. Johnson and R.H. Silsbee, Phys. Rev. B **35**, 4959 (1987)
[8] L. Gravier et al, Phys. Rev. B **73**, 024419 and 052410 (2006)
[9] G.E.W. Bauer et al, Solid State Commun. **150**, 489 (2010).

$$\begin{pmatrix} \vec{j}_c \\ \overleftrightarrow{j}_s \\ \vec{j}_Q \end{pmatrix} = -\frac{1}{\rho^*(1-\beta^2)} \begin{pmatrix} 1 & (\beta/2)(\bar{u}\cdot) & S \\ \beta\,(\bar{u}\otimes) & 1/2 & \beta' S\,(\bar{u}\otimes) \\ ST & (\beta'/2)ST(\bar{u}\cdot) & \rho^*(1-\beta^2)\kappa \end{pmatrix} \cdot \nabla \begin{pmatrix} \phi_c \\ \overleftarrow{\phi}_s \\ T \end{pmatrix} \tag{1.8}$$

Symmetries among linear response coefficients arising from Onsager's reciprocity principle have been explicitly enforced; and a new spin asymmetry coefficient β' for the Seebeck coefficient has been introduced. Of course β' vanishes for a non-magnetic material. On the other hand, Wiedemann-Franz law has not been explicitly enforced, as we want to be able to include in our simulations thermally conducting but electrically insulating materials.

Neglecting for now interface resistances, both electrical and thermal, and consequently neglecting also the corresponding interface dissipation source terms, an approximation that will be relaxed later in the course of the project, the interface boundary conditions to be considered at F/N interfaces reduce to:

$$\begin{cases} \phi_c^{(N)} - \phi_c^{(F)} = 0 \\ \bar{u}.\overleftarrow{\phi}_s^{(N)} - \phi_s^{(F)} = 0 \\ T^{(N)} - T^{(F)} = 0 \end{cases} \qquad \begin{cases} \vec{n}_{(N)}.\vec{j}_c^{(N)} + \vec{n}_{(F)}.\vec{j}_c^{(F)} = 0 \\ \left[\bar{u}\cdot\overleftrightarrow{j}_s^{(N)}\right]\cdot\vec{n}_{(N)} + \vec{n}_{(F)}.\vec{j}_s^{(F)} = 0 \\ \vec{n}_{(N)}.\vec{j}_Q^{(N)} + \vec{n}_{(F)}.\vec{j}_Q^{(F)} = 0 \end{cases} \tag{1.9}$$

$$\left[\bar{u}\times\overleftrightarrow{j}_s^{(N)}\right]\cdot\vec{n}_{(N)} = g_{\uparrow,\downarrow}\bar{u}\times\overleftarrow{\phi}_s^{(N)} \tag{1.10}$$

Equations (1.9) simply state the continuity of the temperature, heat flow, charge potential, charge current, and longitudinal parts of the spin accumulation and the spin current at F/N interface, while (1.10) enforces the abrupt discontinuity of the transverse spin accumulation and spin current which only exist on the N side of the interface. At N/N or F/F interfaces, in the latter case assuming continuity of the magnetization vector, all quantities of interest are simply continuous.

As in the simpler cases of coupled spin-charge transport and thermoelectric system, the linear response equations (1.8) have to be supplemented by continuity equations, which now read:

$$\nabla\cdot\begin{pmatrix} \vec{j}_c \\ \overleftrightarrow{j}_s \\ \vec{j}_Q \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & -1/(2\rho^* l_{sf}{}^2) & 0 \\ -\vec{j}_c.\nabla & -\dfrac{\overleftrightarrow{j}_s.\nabla}{2} & 0 \end{pmatrix} \cdot \begin{pmatrix} \phi_c \\ \overleftarrow{\phi}_s \\ T \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ p_Q^{(0)} \end{pmatrix} \tag{1.11}$$

When compared with (1.7), one shall note the presence of a new dissipation term proportional to the inner product of the spin current with the gradient of its conjugated potential (the spin accumulation). We have also elected to introduce in (1.11) a volume thermal power source term $p_Q^{(0)}$ of unspecified origin, that may allow for instance to model localized heating by a laser beam. What has been left out of the above system (1.11) at this time is the dissipation source term which is proportional to the Gilbert's damping constant and is related to the heat generated by a time dependent magnetization vector. This will be introduced at a later stage when considering the coupling of the transport solver with a dynamic Landau-Lifschitz-Gilbert solver.

One shall also note that we are making in (1.8)-(1.11) the approximation of a single electron temperature independent of the spin degree of freedom, while in general one can introduce the concept of thermal spin accumulation $\overleftarrow{T}_s$. We can possibly relax this approximation later on; even so it is certainly an adequate approximation for most devices of technological interest, as this is expected to break down only at very low temperatures.

3 WEAK FORMULATION

As a first step towards a finite element discrete formulation of the boundary value problem at hands, we want to derive a continuous weak (integral) form from the system of Partial Differential Equations (PDEs) (1.8),(1.11), supplemented by the interface boundary conditions (1.9),(1.10), and yet to be specified external boundary conditions.

3.1 Spatial domain partition

We assume the problem to be stated in a spatial domain $\Omega \equiv \Omega_F \cup \Omega_N \cup \Omega_T$; which has been partitioned between electrically conducting regions, either ferromagnetic (Ω_F) or non-magnetic (Ω_N), and thermally conducting but electrically insulating regions (Ω_T).

From a spin/charge transport standpoint, the problem being stated in $\Omega_F \cup \Omega_N$, the union of all interfaces and outer boundaries, γ_{sc}, is partitioned as:

$$\gamma_{sc} \equiv \gamma^{\phi}_{(F,N)} \cup \gamma^{j}_{(F,N)} \cup \gamma^{0}_{(F,N)} \cup \gamma_{F/F} \cup \gamma_{N/N} \cup \gamma_{F/N} \tag{1.12}$$

With the following definitions:

- $\gamma^{\phi}_{(F,N)}$: The union of all outer boundaries, belonging either to Ω_F or Ω_N, at which an essential (Dirichlet) forced electrical potential boundary condition is enforced. The spin accumulation is forced to vanish at such contacts, which is only correct if the considered contact is far enough from the "active part" of the considered device on the length scale of the spin diffusion length.
- $\gamma^{j}_{(F,N)}$: The union of all outer boundaries, belonging either to Ω_F or Ω_N, at which a Neumann type forced charge current inflow condition is enforced. The spin accumulation is forced to vanish at such contacts, which is only correct if the considered contact is far enough from the "active part" of the considered device on the length scale of the spin diffusion length.
- $\gamma^{0}_{(F,N)}$: The union of all the other outer boundaries, belonging either to Ω_F or Ω_N, at which all current fluxes are assumed to vanish (natural boundary condition).
- $\gamma_{F/F}$: The union of all interfaces between two ferromagnetic regions, at which all quantities of interest are assumed to be continuous.
- $\gamma_{N/N}$: The union of all interfaces between two non-magnetic regions, at which all quantities of interest are assumed to be continuous.
- $\gamma_{F/N}$: The union of all interfaces between a ferromagnetic and a non-magnetic region, at which interface boundary conditions (1.9)-(1.10) apply.

From a thermal transport standpoint, the problem being stated in Ω, the union of all interfaces and outer boundaries, γ_H, is partitioned as:

$$\gamma_H \equiv \gamma^{T} \cup \gamma^{Q} \cup \gamma^{0}_{H} \cup \gamma_{A/B} \tag{1.13}$$

With the following definitions:

- γ^T: The union of all outer boundaries at which an essential (Dirichlet) forced temperature boundary condition is enforced.
- γ^Q: The union of all outer boundaries at which a Neumann type forced heat inflow condition is enforced.
- γ_H^0: The union of all the other outer boundaries, at which the heat flow is assumed to vanish (natural boundary condition).
- $\gamma_{A/B}$: The union of all interfaces, at which the temperature and heat flow are assumed to be continuous.

3.2 Test functions

As it is customary, we introduce now the following function spaces for the test functions to be used:

$$\Xi_{\underset{\sim}{\phi}_c} = \left\{ \underset{\sim}{\phi}_c(\mathbf{r}) / \mathbf{r} \in \Omega_F \cup \Omega_N,\ \underset{\sim}{\phi}_c(\mathbf{r}) \in H^1(\Omega_F \cup \Omega_N) \text{ and } \underset{\sim}{\phi}_c(\mathbf{r}) = 0 \text{ on } \gamma^{\phi}_{(F,N)} \right\} \tag{1.14}$$

$$\Xi_{\underset{\sim}{\overleftarrow{\phi}}_s} = \left\{ \underset{\sim}{\overleftarrow{\phi}}_s(\mathbf{r}) / \mathbf{r} \in \Omega_N, \underset{\sim}{\overleftarrow{\phi}}_s(\mathbf{r}) \in \overleftarrow{H}^1(\Omega_N) \text{ and } \underset{\sim}{\overleftarrow{\phi}}_s(\mathbf{r}) = 0 \text{ on } \gamma_N^{\phi} \cup \gamma_N^j \right\} \tag{1.15}$$

$$\Xi_{\underset{\sim}{\phi}_s} = \left\{ \underset{\sim}{\phi}_s(\mathbf{r}) / \mathbf{r} \in \Omega_N, \underset{\sim}{\phi}_s(\mathbf{r}) \in H^1(\Omega_N) \text{ and } \underset{\sim}{\phi}_s(\mathbf{r}) = 0 \text{ on } \gamma_F^{\phi} \cup \gamma_F^j \right\} \tag{1.16}$$

$$\Xi_{\underset{\sim}{T}} = \left\{ \underset{\sim}{T}(\mathbf{r}) / \mathbf{r} \in \Omega_N, \underset{\sim}{T}(\mathbf{r}) \in H^1(\Omega_T) \text{ and } \underset{\sim}{T}(\mathbf{r}) = 0 \text{ on } \gamma^Q \right\} \tag{1.17}$$

We introduce also the compact standard bracket notation for the L_2 inner product on Ω:

$$\int_{\Omega} d^3r\, \mathbf{A}(\mathbf{r}) \cdot \mathbf{B}(\mathbf{r}) \equiv \langle \mathbf{A}; \mathbf{B} \rangle_{\Omega} \tag{1.18}$$

From (1.11), we derive immediately the following integral relations by projection on the appropriate test functions:

$$\left\langle \underset{\sim}{\phi}_c; \nabla . \vec{j}_c \right\rangle_{\Omega_F \cup \Omega_N} = 0 \tag{1.19}$$

$$\left\langle \underset{\sim}{\phi}_s; \nabla . \vec{j}_s \right\rangle_{\Omega_F} + \left\langle \underset{\sim}{\overleftarrow{\phi}}_s; \nabla . \overleftarrow{\vec{j}}_s \right\rangle_{\Omega_N} = -\frac{1}{2} \left\langle \underset{\sim}{\phi}_s; \frac{\phi_s}{\rho^* l_{sf}^2} \right\rangle_{\Omega_F} - \frac{1}{2} \left\langle \underset{\sim}{\overleftarrow{\phi}}_s; \frac{\overleftarrow{\phi}_s}{\rho^* l_{sf}^2} \right\rangle_{\Omega_N} \tag{1.20}$$

$$\left\langle \underset{\sim}{T}; \nabla . \vec{j}_Q \right\rangle_{\Omega_T} = -\left\langle \underset{\sim}{T}; \vec{j}_c \cdot \nabla \phi_c \right\rangle_{\Omega_F \cup \Omega_N} - \frac{1}{2} \left\langle \underset{\sim}{T}; \vec{j}_s \cdot \nabla \phi_s \right\rangle_{\Omega_F} - \frac{1}{2} \left\langle \underset{\sim}{T}; \overleftarrow{\vec{j}}_s \cdot \nabla \overleftarrow{\phi}_s \right\rangle_{\Omega_N} + \left\langle \underset{\sim}{T}; p_Q^0 \right\rangle_{\Omega_T} \tag{1.21}$$

3.3 Continuous weak formulation

Using Green's first identity, making explicit use of the above introduced spatial domain partitioning and associated definitions, and taking into account the previously stated interface and outer boundary conditions, we obtain quite straightforwardly:

$$\left\langle \nabla \underset{\sim}{\phi}_c ; \vec{j}_c \right\rangle_{\Omega_F \cup \Omega_N} = \left\langle \underset{\sim}{\phi}_c ; \vec{n}_F \cdot \vec{j}_c^{(0)} \right\rangle_{\gamma_F^j} + \left\langle \underset{\sim}{\phi}_c ; \vec{n}_N \cdot \vec{j}_c^{(0)} \right\rangle_{\gamma_N^j} \tag{1.22}$$

$$\left\langle \nabla \underset{\sim}{\phi}_s ; \vec{j}_s \right\rangle_{\Omega_F} - \frac{1}{2} \left\langle \underset{\sim}{\phi}_s ; \frac{\underset{\sim}{\phi}_s}{\rho^* l_{sf}^2} \right\rangle_{\Omega_F} = 0 \tag{1.23}$$

$$\left\langle \nabla \underset{\sim}{\bar{\phi}}_s ; \vec{\bar{j}}_s \right\rangle_{\Omega_N} - \frac{1}{2} \left\langle \underset{\sim}{\bar{\phi}}_s ; \frac{\underset{\sim}{\bar{\phi}}_s}{\rho^* l_{sf}^2} \right\rangle_{\Omega_N} - \left\langle \underset{\sim}{\bar{\phi}}_s ; g_{\uparrow\downarrow} (\bar{u} \times \bar{\phi}_s) \times \bar{u} \right\rangle_{\gamma_{F/N}} = 0 \tag{1.24}$$

$$\begin{aligned} \left\langle \nabla \underset{\sim}{T} ; \vec{j}_Q \right\rangle_{\Omega_T} - \left\langle \underset{\sim}{T} ; \vec{j}_c \cdot \nabla \phi_c \right\rangle_{\Omega_F \cup \Omega_N} - \frac{1}{2} \left\langle \underset{\sim}{T} ; \vec{j}_s \cdot \nabla \phi_s \right\rangle_{\Omega_F} - \frac{1}{2} \left\langle \underset{\sim}{T} ; \vec{\bar{j}}_s \cdot \nabla \bar{\phi}_s \right\rangle_{\Omega_N} \\ = \left\langle \underset{\sim}{T} ; \vec{n} \cdot \vec{j}_Q^{(0)} \right\rangle_{\gamma_Q} - \left\langle \underset{\sim}{T} ; p_Q^{(0)} \right\rangle_{\Omega_N} \end{aligned} \tag{1.25}$$

As expected *forced* charge current densities and heat flows, if any, respectively $\vec{j}_c^{(0)}$ and $\vec{j}_Q^{(0)}$, appear on the right hand side of (1.22) and (1.25).

Now we can use the linear response relations (1.8) to eliminate the currents from the integral equations (1.22)-(1.25), leading to the following weak form expressed only in terms of the unknown potentials and temperature, and associated test functions:

$$\begin{aligned} \left\langle \nabla \underset{\sim}{\phi}_c ; \frac{\nabla \phi_c}{\rho^* (1-\beta^2)} \right\rangle_{\Omega_F \cup \Omega_N} + \left\langle \nabla \underset{\sim}{\phi}_c ; \frac{\beta \nabla \phi_s}{2\rho^* (1-\beta^2)} \right\rangle_{\Omega_F} + \left\langle \nabla \underset{\sim}{\phi}_c ; \frac{S \nabla T}{\rho^* (1-\beta^2)} \right\rangle_{\Omega_F \cup \Omega_N} \\ = - \left\langle \underset{\sim}{\phi}_c ; \vec{n}_F \cdot \vec{j}_c^{(0)} \right\rangle_{\gamma_F^j} - \left\langle \underset{\sim}{\phi}_c ; \vec{n}_N \cdot \vec{j}_c^{(0)} \right\rangle_{\gamma_N^j} \end{aligned} \tag{1.26}$$

$$\left\langle \nabla \underset{\sim}{\phi}_s ; \frac{\beta \nabla \phi_c}{\rho^* (1-\beta^2)} \right\rangle_{\Omega_F} + \left\langle \nabla \underset{\sim}{\phi}_s ; \frac{\nabla \phi_s}{2\rho^* (1-\beta^2)} \right\rangle_{\Omega_F} + \left\langle \nabla \underset{\sim}{\phi}_s ; \frac{\beta' S \nabla T}{\rho^* (1-\beta^2)} \right\rangle_{\Omega_F} + \frac{1}{2} \left\langle \underset{\sim}{\phi}_s ; \frac{\underset{\sim}{\phi}_s}{\rho^* l_{sf}^2} \right\rangle_{\Omega_F} = 0 \tag{1.27}$$

$$\left\langle \nabla \underset{\sim}{\bar{\phi}}_s ; \frac{\nabla \bar{\phi}_s}{2\rho^* (1-\beta^2)} \right\rangle_{\Omega_N} + \frac{1}{2} \left\langle \underset{\sim}{\bar{\phi}}_s ; \frac{\underset{\sim}{\bar{\phi}}_s}{\rho^* l_{sf}^2} \right\rangle_{\Omega_N} + \left\langle \underset{\sim}{\bar{\phi}}_s ; g_{\uparrow\downarrow} (\bar{u} \times \bar{\phi}_s) \times \bar{u} \right\rangle_{\gamma_{F/N}} = 0 \tag{1.28}$$

$$\left\langle \nabla \underset{\sim}{T}; \frac{S T \nabla \phi_c}{\rho^*(1-\beta^2)} \right\rangle_{\Omega_F \cup \Omega_N} + \left\langle \nabla \underset{\sim}{T}; \frac{\beta' S T \nabla \phi_s}{2\rho^*(1-\beta^2)} \right\rangle_{\Omega_F} + \left\langle \nabla \underset{\sim}{T}; \kappa \nabla T \right\rangle_{\Omega_T}$$

$$- \left\langle \underset{\sim}{T}; \frac{\nabla \phi_c \cdot \nabla \phi_c}{\rho^*(1-\beta^2)} \right\rangle_{\Omega_F \cup \Omega_N} - \left\langle \underset{\sim}{T}; \frac{\beta \nabla \phi_s \cdot \nabla \phi_c}{2\rho^*(1-\beta^2)} \right\rangle_{\Omega_F} - \left\langle \underset{\sim}{T}; \frac{S \nabla T \cdot \nabla \phi_c}{\rho^*(1-\beta^2)} \right\rangle_{\Omega_F} \tag{1.29}$$

$$- \frac{1}{2} \left\langle \underset{\sim}{T}; \frac{\beta \nabla \phi_c \cdot \nabla \phi_s}{\rho^*(1-\beta^2)} \right\rangle_{\Omega_F} - \frac{1}{2} \left\langle \underset{\sim}{T}; \frac{\nabla \phi_s \cdot \nabla \phi_s}{2\rho^*(1-\beta^2)} \right\rangle_{\Omega_F} - \frac{1}{2} \left\langle \underset{\sim}{T}; \frac{\beta' S \nabla T \cdot \nabla \phi_s}{\rho^*(1-\beta^2)} \right\rangle_{\Omega_F}$$

$$- \frac{1}{2} \left\langle \underset{\sim}{T}; \frac{\nabla \overleftarrow{\phi}_s \cdot \nabla \overleftarrow{\phi}_s}{2\rho^*(1-\beta^2)} \right\rangle_{\Omega_N} = - \left\langle \underset{\sim}{T}; \vec{n} \cdot \vec{j}_Q^{(0)} \right\rangle_{\gamma^Q} + \left\langle \underset{\sim}{T}; p_Q^{(0)} \right\rangle_{\Omega_T}$$

The integral equations (1.26)-(1.29), supplemented by essential boundary conditions on $\gamma^{\phi}_{(F,N)}$ and γ^{T}, constitute a well-posed continuous weak formulation of the boundary value problem associated with a general 3D spin caloritronic device at the chosen level of physical model.

One shall realize that the dissipation terms in (1.29) make the problem explicitly *nonlinear*, while other nonlinearities may arise from the temperature dependence, if considered, of any of the physical material parameters.

4 FINITE ELEMENT IMPLEMENTATION

We refer to standard textbooks on the finite element method for a detailed description of the steps involved in the discretization by finite elements of a continuous weak formulation such as (1.26)-(1.29). We will just provide here a quick overview, stating primarily the specific implementation choices that have been made.

First order P1 type (linear Lagrange) 3D tetrahedral finite elements have been chosen for the interpolation of the primary degrees of freedom (electrochemical potential, spin accumulation and temperature), and test functions.

As planned, the actual implementation of the targeted transport equation solver was undertaken by In Silicio as a prototype extension to the previously developed (in part with the support of the previous FP6 project DYNAMAX), and now commercially available in its version 1.1, spintronics simulation software SpinFlow 3D.

This implementation effort has resulted in the creation of two new solver software classes, LinSpinCalo (linear spin caloritronic solver) and NLinSpinCalo (nonlinear spin caloritronic solver).

LinSpinCalo solves for a linearized version of the discrete system derived from (1.26)-(1.29), meaning all material parameters are temperature independent, and all nonlinear dissipation source terms are removed from (1.29). The primary use of LinSpinCalo is to generate a starting point for the nonlinear iterative solver implemented in NLSpinCalo.

NLSpinCalo solves for the full nonlinear discrete system derived from (1.26)-(1.29), with full support for arbitrary temperature dependence of all material parameters, possibly using a solution previously obtained by LinSpinCalo as starting point. The *direct iteration method* (also known as the Picard's method) has been implemented to iteratively solve the nonlinear problem at hands.

As for any of the previously developed solvers currently part of the SpinFlow 3D platform, the low level parts performing the computationally intensive discrete problem assembly and resolution is coded in C/C++, with for the resolution part links into highly optimized standard linear algebra libraries (SPARSKIT, with a future transition planned to PETSC). High level control scrip files enable to select among a broad choice of pre-conditioning (ILU, ILUk, ILUTP,…) and linear iterative solver algorithms (Conjuguate Gradients, GMRES, DGMRES…), and set the corresponding control parameters.

Also conforming to the general design choices made for the pre-existing SpinFlow 3D platform, the exposed software interface has been implemented as a Python interface, which allows taking advantage of all the flexibility and power of Python as a programming language to script and automate complex simulation sequences.

Thanks to this choice of building up on top of the pre-existing SpinFlow 3D platform, both solvers are already interoperable with some of the pre-existing ones. For instance, an equilibrium micro-magnetic configuration for the device of interest can be obtained from the pre-existing StationaryLLG solver, and then imported to initialize the magnetic configuration to be considered by either LinSpinCalo or NLSpinCalo.

5 CONCLUSION

The two new solvers LinSpinCalo and NLSpinCalo have been fully implemented and are functional. They materialize the delivery on time of deliverable D1.1.

As planned, we are now entering a phase of detailed numerical testing, with later on cross validation planned with the CRMT3D based solver developed by the CEA node, and planned comparisons of numerical simulation results against experimental results generated within and outside the MACALO consortium.

We have started to set up for that purpose test device models. One can see in Fig.1 an example of such model, which consists in a type of non-local planar spin valve device. Different kind of electrical and thermal loads can be applied to the model.

A summary of preliminary numerical results will be provided as part of the WP 1 presentation during the 12 month project review on October 6, 2011.

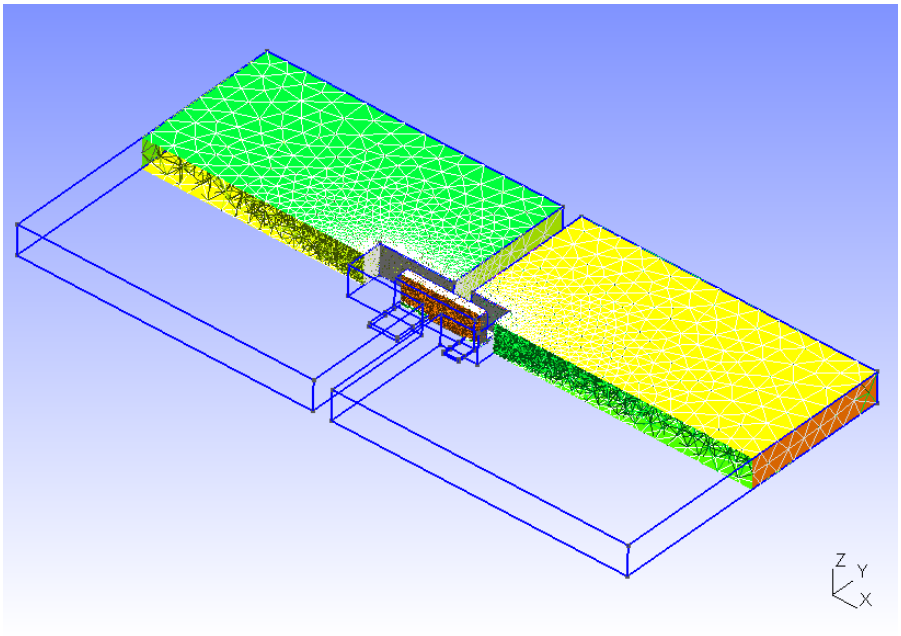

Fig.1 – Example of test device structure numerical model set up for detailed validation of newly implemented solvers. Two ferromagnetic elements connected by a non-magnetic conducting element, with contact “pads” allowing to apply electrical and thermal loads. The computational mesh contains of the order of 300 k finite elements (tetrahedrons).