Analysis of the perspectives of multiscale simulation of devices and circuits

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Summary

- Structure and scope of the report that is being prepared for Mult.Eu.Sim on multi-scale device and circuit modeling
- Procedure followed to create a document representative of a shared view
- Summary of the main contents and the main issues that have been raised
- What may be interesting for the industry
- Conclusions

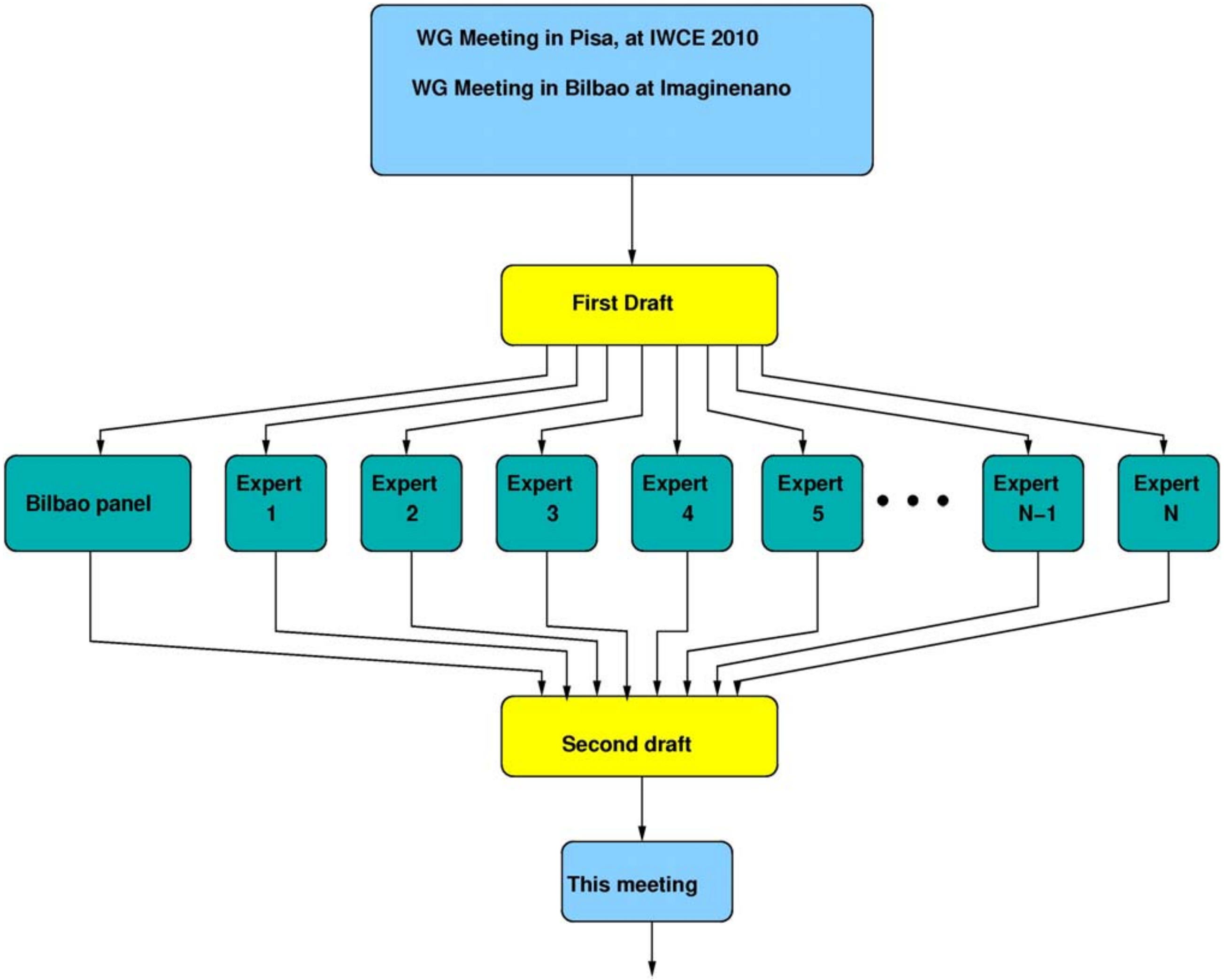
Scope of the document

- **The scope of the document has been the role of modeling and, in particular, of multi-scale modeling of devices and circuits in the development of nanoelectronics in the near future**
- **We have focused on the contribution that modeling can provide to developers of new technologies, device and circuit designers, and other researchers in the field**
- **We have tried to understand what the industry currently lacks and what it will find valuable in the next few years**

Structure of the document

- **The structure of the document is relatively straightforward:**
  - **Discussion of the relationship between device and material modeling and of the multi-scale structure that is involved**
  - **A few case studies**
  - **Relevance of high-performance computing and computational architectures**
  - **Role of physics based modeling**
  - **Simulation of time-dependent behavior**
  - **Relationship between device and circuit modeling**

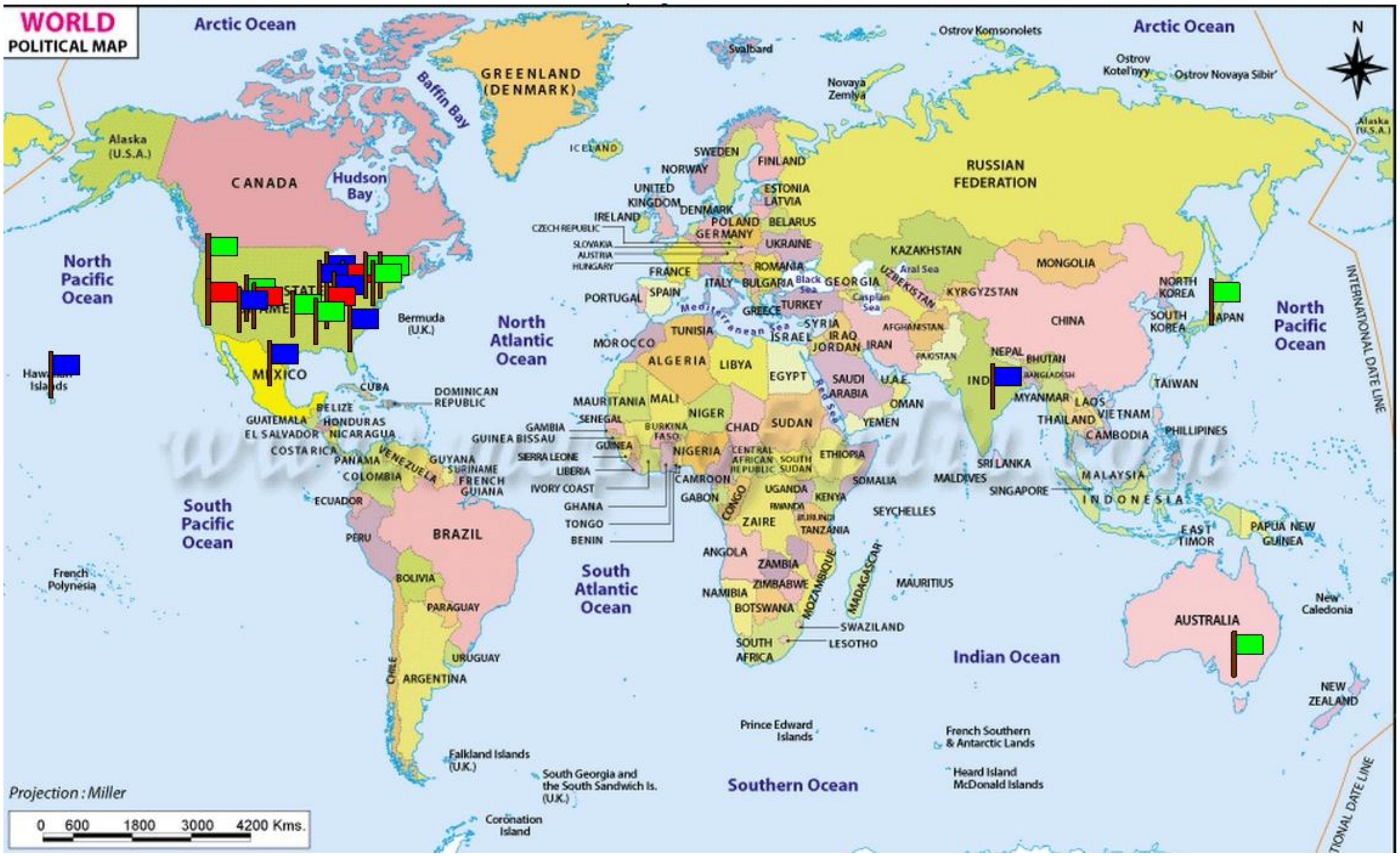
Origin of the document



Feedback from Europe

The response has been overwhelming, with comments and new contributions that have significantly enlarged and improved the document

Feedback from outside Europe



Materials and device modeling

- **It is recognized that, as device sizes are scaled down, the gap between the simulation of materials and that of devices is closing and in some cases they already overlap**
- **Multi-scale approaches are needed because ab-initio methods cannot directly allow treatment of complete devices and circuits**
- **However significant progress has been made with the development of linear-scaling codes, such as ONETEP and SIESTA**
- **The requirement of self-consistency makes the computational burden very heavy**

Organic Semiconductors

- Disorder plays an important role in transport in organic semiconductors, and this adds to the computational complexity of its simulation
- Recent multi-scale methods have been developed, which include treatment of polaron transport using first principles and a Kubo approach for quantum transport
- Open issues are the interplay of impurity scatterings with phonons and the transport regime as a function of temperature

Nanowire transistors

- Another field in which multi-scale modeling is expected to represent offer substantial contributions is that of nanowire transitors and of the circuits based on them
- It has been demonstrated that a fully-functional “gate-all-around” transistor based on a silicon nanowire can operate correctly down to a channel length of 3 nm
- An explicit quantum-mechanical description of the atomic scale structure has enabled calculations showing that operation is possible down to a diameter of 1 nm

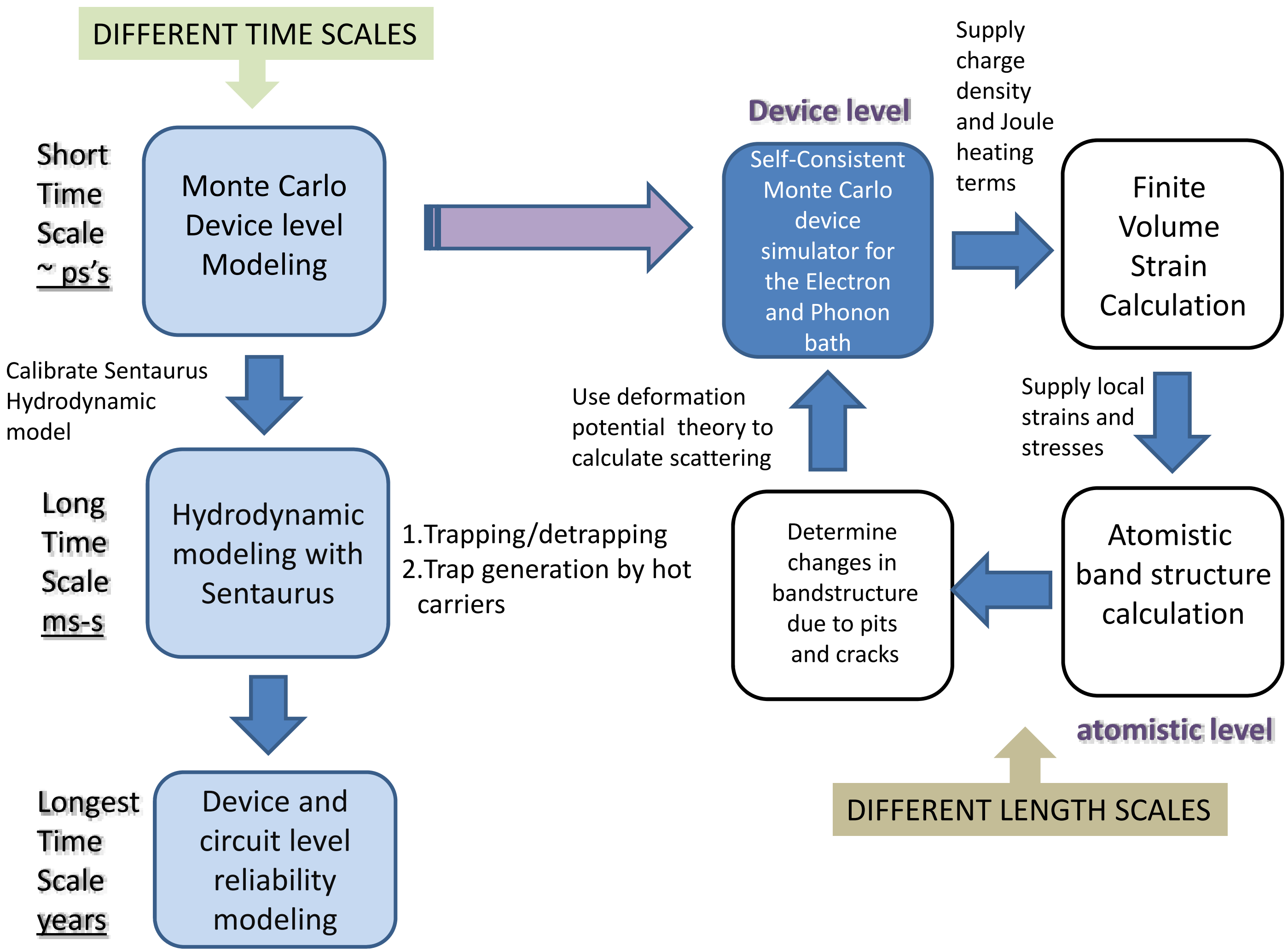
Interactions between nanostructures and biological molecules

- **The comparable length scale of biomolecules and currently manufacturable semiconductor nanostructures open a completely new horizon of possibilities**
- **This is true both in terms of exploiting the properties of biomolecules to help develop bottom-up fabrication approaches and of taking advantage of their recognition and biocatalytic properties to create "lab-on-a-chip" systems**
- **Key to these studies is developing a multi-scale simulation framework that can handle the large simulations needed to atomistically describe the combined nanowire/biomolecule system, yet be able to treat the electronic structure of these systems to describe interactions with light and electronic transport phenomena**

Current collapse in GaN HEMTs

- GaN HEMTs are very promising devices for high-power, high-frequency applications, due the ability to operate safely at temperatures much higher than other semiconductor devices
- However, there is still a reliability problem, because they often fail in a relatively short time if operated at high power levels
- In particular, efforts are ongoing to understand the reasons of such a failure and of the "current collapse" effect observed after the application of an elevated drain-to-source voltage

Need for a multi-scale treatment of current collapse



Role of high-performance computing

- The use of High Performance Computing is essential for achieving advances in frontier developments in the fields of first-principles calculations and multi-scale methodologies.
- There is therefore a need for the usage of supercomputers, but the power of current supercomputers is not expected to become available to the majority of users in the foreseeable future
- If we want the new hierarchies of multi-scale tools to be useful for device and circuit designers, they must run efficiently on widely available machines

Computational equipment (I)

- **The best performance to cost ratio is currently achieved with GPUs (Graphic Processor Units) that were originally developed to deliver optimized 3D graphics but that, due to the massively parallel structure, can be exploited also for the solution of challenging numerical problems**

- **The acceptance of GPUs for HPC is reflected by the fact that leading edge machines in the top 500 supercomputers contain GPUs**

- **GPUs can handle hundreds of concurrent lightweight threads compared to the much smaller number of more complex threads that can be treated with CPUs**

Computational equipment (II)

- High degrees of parallelism (although at least oen or two orders of magnitude below those of GPUs) can be achieved also with more conventional multi-core CPUs
- The choice between GPUs and CPUs depends on the specificity of the algorithm and a well-balanced, general-purpose machine should contain the right mix of GPUs and CPUs
- Extreme parallelization requires a lot of work on the software development front, from which very significant speedups can result

Predictive capabilities of physics-based modeling

- There are success stories about the predictive capabilities of advanced numerical simulations
- One example is the prediction, resulting from an accurate interface model, that the TMR (Tunneling Magneto Resistance) ratio was going to improve dramatically when the dielectric was crystalline instead of amorphous
- Today TMR-based heads are equipping virtually all hard disks and have allowed a significant improvement in data storage density

Time-domain simulation

- Time-domain behavior of nanodevices has received so far much less attention compared to DC transport
- There is now a growing interest in the behavior as a function of frequency and in the noise characteristics of nanodevices, which requires an understanding of time-dependent transport
- There are a few proposals in the literature that could be developed into full-fledged multi-scale tools, but some effort is needed, also in collaboration with experimental groups

Device and circuit levels

- At the nanoscale the distinction between device modelling and circuit modelling starts to vanish
- One of the main reasons is apparent in single-electronics: a SPICE description fails unless the capacitances at the nodes corresponding to the devices terminals are not significantly larger than the internal device capacitances
- If a model based on the I-V characteristics at the terminals fails, traditional circuit simulation cannot be performed and different approaches, based on multi-scale techniques have to be developed

What is interesting for the industry?
(statements collected from industry representatives)

- **The industry is interested in simulation tools that can tell when something is not going according to intuition rather than in tools that are capable of very accurate predictions**
- **The industry needs new tools very soon, because there are a lot of effects becoming important also in current generations of CMOS devices that cannot be properly dealt with existing software**
- **The industry needs simulation tools that are very simple to use and in which all challenging setup tasks are performed automatically**

Conclusions

- **Multi-scale modeling is the way to go in the next future for material-device-circuit simulation**
- **Big challenges are represented by the computational burden, the accessibilty to designers, the validation with experimental tests**
- **Future multi-scale tools will need to exploit all the computational power of low-cost solutions (such as desktops integrated with GPU boards)**
- **A shared view of the device and circuit modeling community will be available in the report that is being prepared**

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