EMMC Roadmap Meeting

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Supply and Industrial Use of Materials Modelling Software

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Outline

- The Key Suppliers of materials modelling software
  - Discrete (e/a/m) - Continuum (c)
  - Academic – Commercial
- Industrial Users
  - Chemical
  - Electronic
  - Automotive and aerospace
  - Oil, gas, renewable energy
  - Other
- Key Roadblocks
- Conclusions and recommendations from SOW perspective

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Commercial modelling companies

Employees	Atomistic	Continuum
<20	Scienomics (EU) Culgi (EU) Gaussian (US) SCM (EU)	Intuition software (AP)
20-100	Materials Design (EU/US) QuantumWise (EU) Schrodinger (US) Tripos (US)	Granta (EU)
100<	Dassault systems (EU)	Ansys (US) Comsol (EU/US) Synopsys (US) Dassault systems (EU)

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Sample Atomistic and Continuum Modelling Software

	Atomistic		Continuum	
	Academic-Gov	Commercial	Academic-Gov	Commerical
Simulation Engines	VASP (EU) CASTEP (EU) Quantum Espresso (EU) Wien2k (EU) SIESTA (EU) FHI-aims (EU) Abinit (EU) Turbomole (EU) MOPAC (US) NWChem (US) Lammps(US) Gulp (US)	ATK (EU) ADF (EU) DMOL (EU) Gaussian (US) Jaguar (US)	OpenFoam Agros2D CalculiX Deal.II DUNE Elmer FEATFLOW FEATool FEAP FEB OOF (USA)	Ansys (US) Abaqus (EU) COMSOL (EU/US) ADINA Advance Design Sentaurus LS-Dyna Nastran VisualFEA (AP)
Front ends	ASE (EU) PYMATGEN (US) PyMD VMD Molden	VNL-ATK (EU) Materials Studio (EU) ADF-GUI (EU) MAPS (EU) Schrodinger (US) Gaussview (US) Culgi (EU) MEDEA (EU/US)	Paraview/VTK	Ansys (US) Abaqus (EU) COMSOL (EU/US) Sentaurus workbench (US) Simscale VisualFEA (AP) Granta (EU)

http://asdn.net/asdn/links/software.php#design

https://en.wikipedia.org/wiki/List_of_finite_element_software_packages

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Industrial Users

- **Chemical** – major chemical companies have modeling groups since the 1980's using discrete models; modelling of solid state systems (heterogeneous catalysis) started later; smaller chemical companies are still in the process of adopting discrete models
- **Electronic** – leading electronics companies have been pioneering discrete models on the electronic and atomistic levels since the 1970's (IBM, NEC, Bell Labs); today major players like Intel, Samsung, Fujitsu, Panasonic, TSMC use commercial e/a software
- **Automotive** – leading companies like Toyota, Honda, GM have been using e/a modelling in-house since several decades; European car companies are in the process of adopting e/a modelling
- **Oil, gas, energy** – leading companies like Shell and ExxonMobil have in-house modelling groups using e/a models; government supported research organizations (IFPEN, Mexian Petroleum Institute) support industrial efforts
- **Other** – xxx

Large companies have dedicated modelling groups using both commercial as well as academic discrete modelling software; smaller companies need to rely more on commercial software or on collaborations with universities.

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Key Roadblocks – Discrete Modelling Software

1. **Intrinsic limitations**
   - The gap between actual industrial materials and the current capabilities of e/a methods remains very large. The various methods remain disconnected.
2. **Lack of investment**
   - The investment to transfer academic knowledge into commercial software tools is too low
3. **Mismatch between academic and industrial objectives**
   - Software innovation by academic groups serve primarily the objectives of academic research (“novel”, “exotic”) while industrial objectives are often mundane (corrosion, failure mechanisms)
   - Often the academic research is focused on promoting a specific tool, rather than progressing the field
   - Academic groups in Europe use software licenses (GPL) incompatible with industrial exploitation
4. **Reluctance of Technology Managers**
   - Management wants to see prove of ROI
   - ….

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Conclusions

1. Discrete models are well established in the major chemical companies (BASF, Dupont, Dow, Sumitomo Chemical) since several decades. The expansion to smaller chemical companies is slow.
2. The use of e/a/m modelling in industries dealing with solid state materials is emerging
3. The key bottlenecks are
   - Shortcomings in the intrinsic capabilities
   - Lack of industry-ready integrated, standardized, interoperable software solutions
   - Lack of trained translators
   - Coupling between the atomistic and the continuum scales
4. Government investments are often guided by academic objectives, not progressing the transfer of modelling software to industrial endusers
5. Continuum modelling is well established with a few large commercial software owners. Discrete models is less established with many scattered small commercial and academic software owners.
6. Strong academic community in Europe within discrete models.

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Recommendations

1. **Training**
   - Universities should even more emphasize training e/a/m modelling
   - Workshops for industrial engineers
   - Workshops for industrial R&D leaders and decision makers
2. **Software**
   - Recognition that software for academic research and software for industrial product and process development have different objectives, both valuable for society, but different.
   - Support academic research that focus on progressing the entire infrastructure, thus of general use to both academic and commercial players, i.e. method development or software libraries which are easy to integrate. Good examples are LibXc, ELPA, PEXSI, LAPAC, …
   - Fund software projects with a solid business model, i.e. are profit generating after the project period by offering a valuable service to the industry.