Efficient electromagnetic and multiphysics simulation - from nanomaterials to macro devices

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Aim

• Review the EM and multiphysics simulation tool, Opera

• Give an overview of its utility
  – In both nano-scale and macro-scale devices

• Introduce a new capability in the software
  – Magnetron simulation
But first…

Vector Fields Software

• **Who we are**
  - part of Cobham plc, a UK aerospace company

• **What we do**
  - Provide electromagnetic design software, consultancy and application expertise

• **When**
  - Founded 1984 as a spin out from the UK Rutherford Appleton lab
    • Aim of commercializing the EM finite element software developed at RAL

• **Where**
  - UK (main office) - Oxford, US office - Chicago
  - Distributors worldwide
Opera

- Multiphysics simulator - EM / thermal / stress
  - Static, harmonic and transient
  - Coupled motion
  - 2D / 3D Finite element solver modules
  - GUI based Modeller and Post-Processor
  - Circuit coupling
    - Built-in circuit editor and simulator
  - System coupling
    - To Simulink®
- Optimizer
- CAD import/export

Solvers
- TOSCA, ELEKTRA, SCALA, CARMEN, SOPRANO, TEMPO, DEMAG, QUENCH, MULTIPHYSICS

Modeller
Pre-Processor
Post-Processor

ELECTROMAGNETICS
CIRCUITS
THERMAL
STRESS
**Applications**

- Mainly static/low frequency:
  - Motors and Generators
  - Actuators and Sensors
  - Transformers
  - MRI / NMR
  - Magnetic Shielding
  - NDT Equipment
  - Magnetic Levitation
  - Induction heating
  - Signatures
  - X-Ray tubes
  - Electron Lithography
  - Particle Accelerators
  - Ion Sources
  - Magnetrons
  - Lightning threat
  - Lightning strike

- Users in universities, research labs and commercial organizations
  - Customer base ~1/3 each North America, Europe, RoW
Typical Opera application area – MRI

• **Opera simulation tasks**
  - Magnet design
    • High quality fields $\sim 1 \times 10^6$ or better
  - Screening design
    • Wide dynamic range
      - $\sim 10^5$ - a few tesla to less than 1 gauss
  - Quench mitigation
    • Highly non-linear heat capacity
    • Rapid propagation of temperature front
    • Fast rate of change of current
  - Stress analysis
    • Lorentz forces from induced eddy currents
      - Can damage the coils and structural components
Nanoparticles for drug delivery

- **Many drugs have high toxicity**
  - Aim to target the drug
    - lowers whole body dose and unwanted side effects
- **Can conceive of several types of targeting**
  - Design the drug to be specific
    - For example recognize antigens or receptors expressed only by the tumour cells
  - Design the delivery system to concentrate the dose in the required location
- **For the latter, use magnetic particles**
  - Typically iron oxide
  - Add a functionalized coating and load with the drug
  - Direct and retain in required location by a magnetic field gradient
Nanoparticles for drug delivery

- **Issue - particles tend to agglomerate**
  - If unchecked can lead to embolism
    - Two causes
      - Surface effects and remanent magnetism
    - Remedy the former using a surfactant coating
    - For the latter need to ensure that the remanent magnetism is zero

- **Core material cannot be ferromagnetic**
  - Always non-zero remanence

- **Paramagnetism generally too weak**

- **Fortunately particle size gives the solution**
Nanoparticles for drug delivery

- **If particles are small enough**
  - $<\sim 100\text{nm}$ diameter

- **No long-range order**
  - Energy required to flip spin states $< \text{thermal energy available at room temperature}$
  - A bulk ferromagnetic material appears to be paramagnetic
  - But with much larger magnetization
    - Super paramagnetic
    - Particle locomotion and retention practicable

- **Currently being modelled in Opera**
  - Forces on particles
  - Motion in viscous fluid

Nanoparticles for hyperthermal therapy

- An alternative or complement to drug therapy
- Target the location of lossy magnetic particles
  - Using field gradient
- Apply a time-varying field
  - Temperature of the particles rises
    - Mainly hysteresis loss
    - Cell death at ~43C
- Most phases are amenable to modelling in Opera
  - Particle locomotion
  - Retention
  - Power dissipation
  - Temperature change
Space charge simulation in Opera

- **Modelling of particle beams**
- **Fully relativistic simulation with**
  - Electrostatic fields
  - Magnetic fields
    - Beam self-magnetic fields
    - External magnetic fields
  - Space charge
  - Emission current
  - Dielectric charging
- **Fast and accurate**
  - Not a PIC code

* courtesy of Thin Film Consulting, Longmont, Colorado, USA
Nanostructures as particle emitters

- **Emission relies on field effect**
  - High field gradients
    - Emission from cold cathodes
  - Model as Fowler-Nordheim or Schottky emitters
  - Maintain adequate mesh quality around the tip
Nanostructures as particle emitters

- **Simple arrays can be represented physically**
- **Practical displays require very large arrays**
  - These can also be simulated
    - Typically use unit cell and appropriate EM boundary conditions
    - Particle reflections modelled by secondary particle generation
Space charge and particle analysis

- **Approaches to analysis**
  - Analytic methods
    - Generally, accurate if reasonable simplifications can be made
    - Restricted to a limited set of geometries, materials etc
  - Numerical methods
    - Allow complex geometry and can capture material behaviour - especially non-linearity
    - Can give additional physical insight

- Two common approaches to numerical modelling
  - PIC
    - Accurate, but computationally intensive
  - Particle tracking
    - Accurate, less computationally demanding - faster
Plasma emitter

- **Provides capability to simulate magnetron sputtering**
  - Self-consistent magnetron plasma simulation
  - Arbitrary geometry, electric and magnetic configurations
  - Particle, electrostatic and magnetostatic solutions
  - Compatible with the standard Optimizer package

- **Developed in association with Thin Film Consulting**
Plasma emitter

- **Simulations provide**
  - Electrostatic and magnetostatic potentials and fields
  - Charge density
  - Particle tracks, beam parameters and profiles
    - Momenta, energy, TOF, current etc

- **Allows evaluation of**
  - Target erosion profile
  - Target utilization
  - Deposition profile
  - Power deposition and thermal load
  - Losses to walls and structure
Magnetron simulation sample results comparison

- Validation against several different magnetron designs
  - Teer Coatings Ltd.
  - Utilization
    - Simulated 35.73%
    - Measured 35.30%

Plasma electrons above the target

Erosion profile - measured and simulated

Sputtered particle distribution at the substrate
Magnetron simulation sample results comparison

- **Validation against several different magnetron designs**
  - Colorado Concept Coatings LLC.
  - Utilization
    - Simulated 25.90%
    - Measured 26.44%

Erosion profile – measured and simulated

Ar ion beam profile at the substrate

Sputtered particle distribution at the substrate
Magnetron coater simulation

- **Simulations are computationally efficient**
  - Allows simulation of coaters
    - Open and closed configurations
    - Balanced and unbalanced magnetrons
Acknowledgements

- Thin Film Consulting, Longmont, Colorado, USA
  - Software validation

- Teer Coatings Ltd., Miba Coating Group, Worcestershire, UK
  - Device specifications and measured data

- Colorado Concept Coatings LLC, Loveland, Colorado, USA
  - Device specifications and measured data
Finally

• **Opera applications, general**
  - operafea.com

• **Opera space-charge applications**
  - charged-particle-devices.com