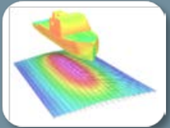
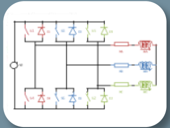


FEA ANALYSIS

General-purpose multi-physics design and analysis software for a wide range of applications

OPTIMIZER

Automatically selects and manages multiple goal-seeking algorithms



INTEROPERABILITY

Built-in circuit modelling and interfaces to leading CAD packages

SERVICE

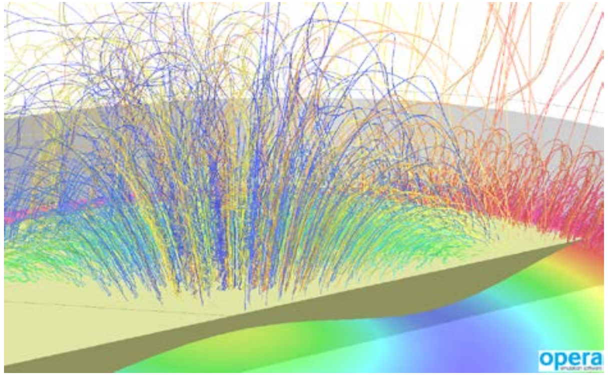
Technical support, training and consultancy services available for software usage and applications

Efficient electromagnetic and multiphysics simulation - from nanomaterials to macro devices

Mike Hook
Vector Fields Software

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



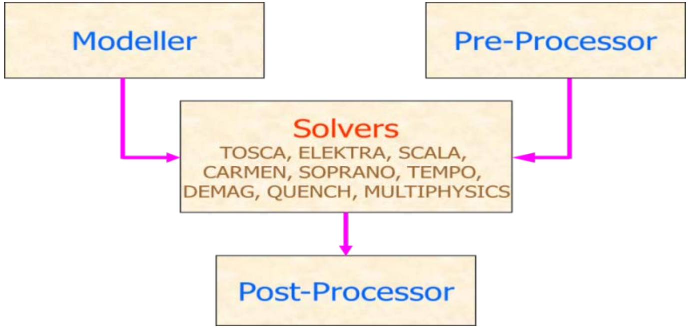
But first...

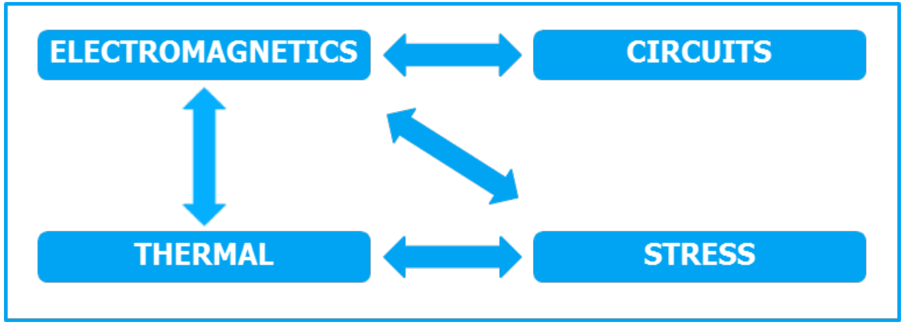
Vector Fields Software

- **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

- **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



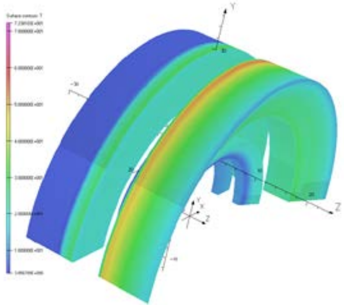


Opera

- **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

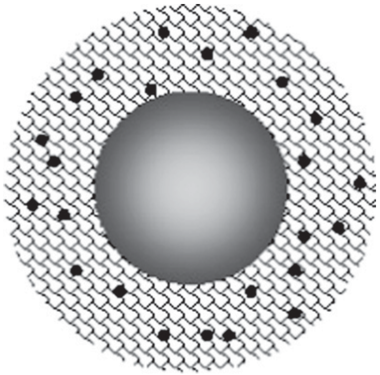
Typical Opera application area – MRI

- **Opera simulation tasks**
  - Magnet design
    - High quality fields ~1 in 10^6 or better
  - Screening design
    - Wide dynamic range
      - ~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

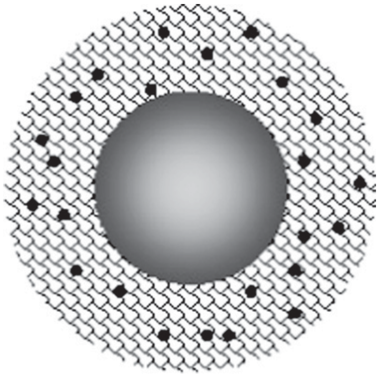


Nanoparticles for drug delivery

- **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

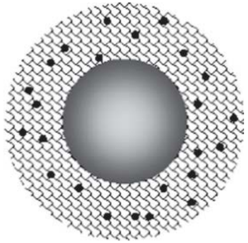
- **Core material cannot be ferromagnetic**
  - Always non-zero remanence
- **Paramagnetism generally too weak**

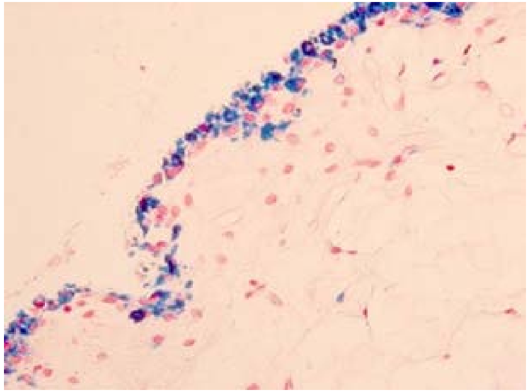
- **Fortunately particle size gives the solution**



Nanoparticles for drug delivery

- **If particles are small enough**
  - <~100nm diameter
- **No long-range order**
  - Energy required to flip spin states < 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





Hofmann-Amtenbrink et al, Nanostructured Materials for Biomedical Applications, 2009

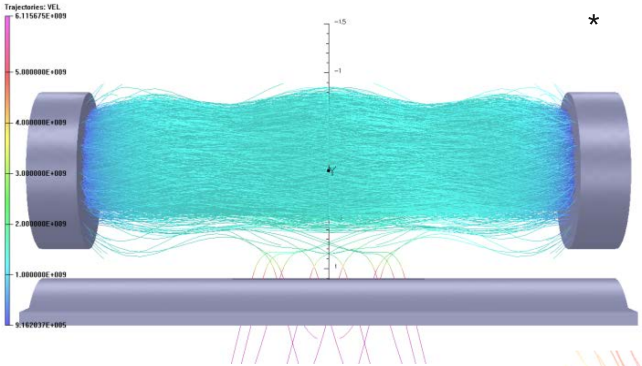
Nanoparticles for hyperthermal therapy

- **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

COBHAM

- **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



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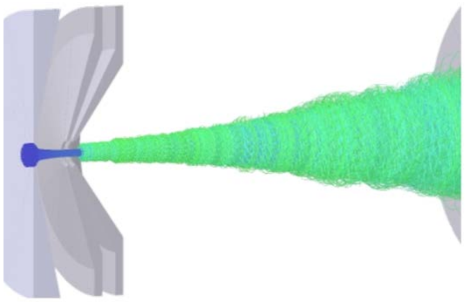

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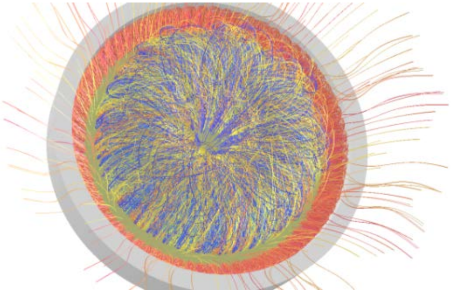
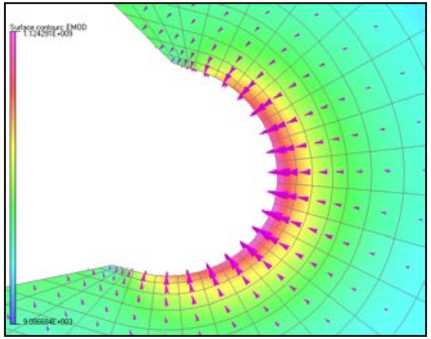
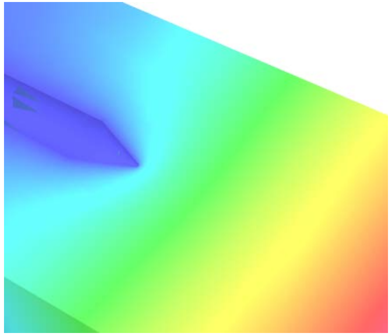


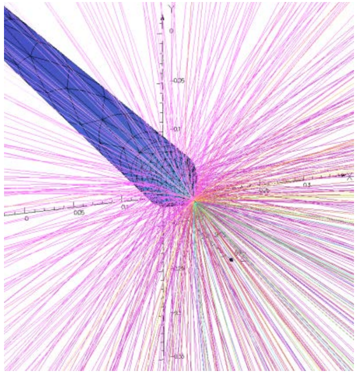
* courtesy of
Thin Film Consulting
Longmont, Colorado, USA

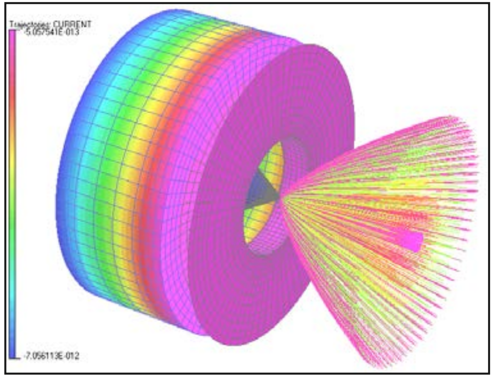
Nanostructures as particle emitters

- **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



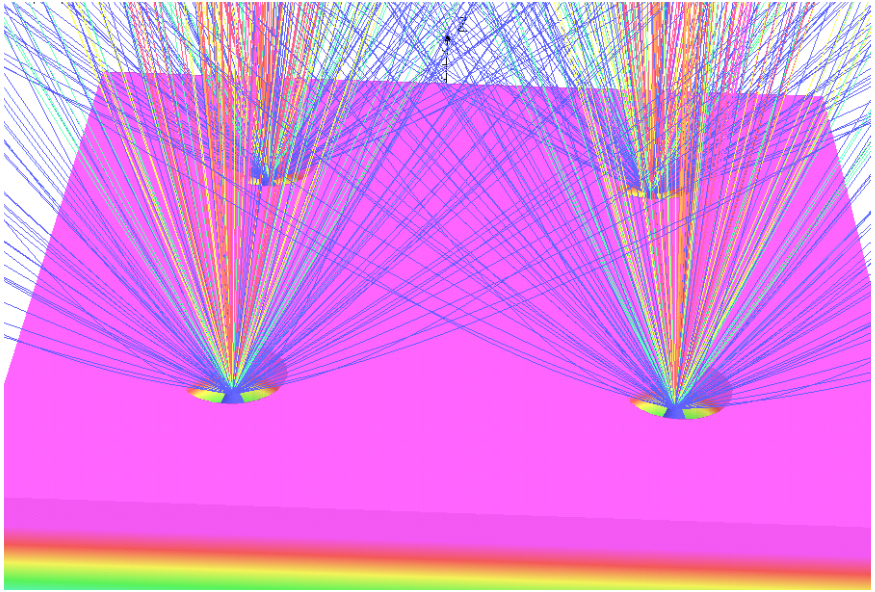






Nanostructures as particle emitters

- **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

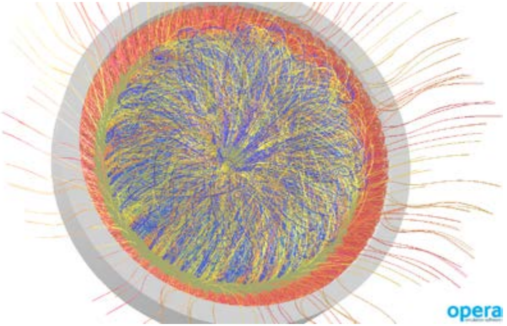


Space charge and particle analysis

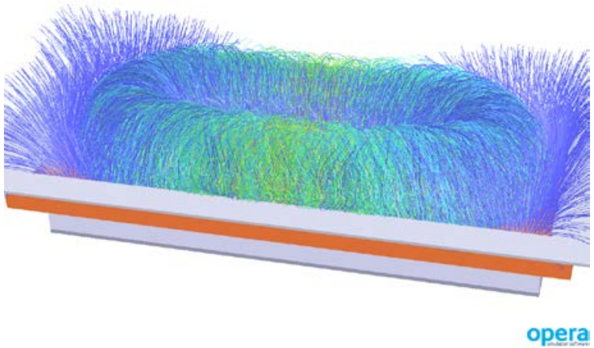
- **Approaches to analysis**
  - Analytic methods
    - Generally, accurate if reasonable simplifications can be made
    - Restricted to a limited set of geometries, materials etc
  - Numerical methods
    - Allow complex geometry and can capture material behaviour - especially non-linearity
    - Can give additional physical insight
    - Two common approaches to numerical modelling
      - PIC
        - Accurate, but computationally intensive
      - Particle tracking
        - Accurate, less computationally demanding - faster

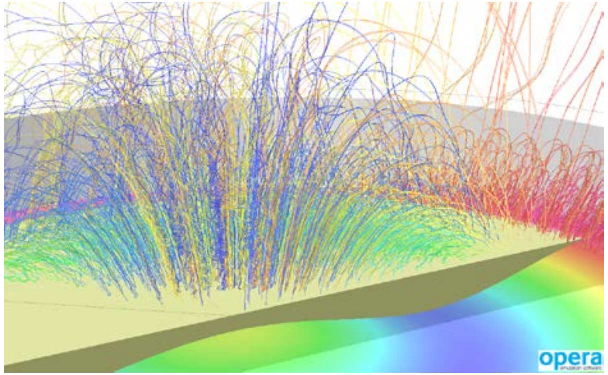
Plasma emitter

- **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



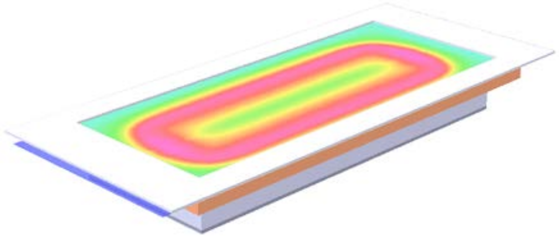
- **Developed in association with Thin Film Consulting**

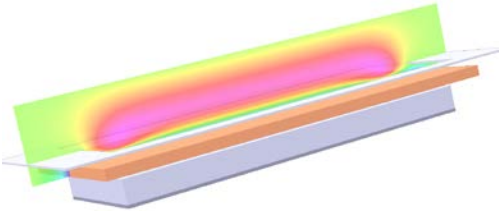




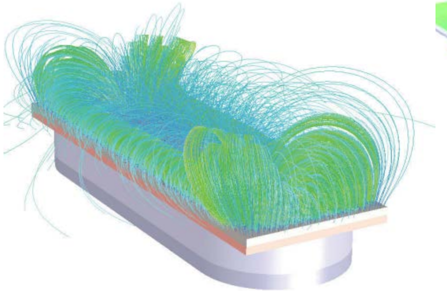
Plasma emitter

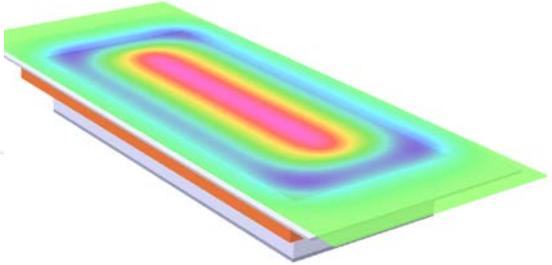
- **Simulations provide**
  - Electrostatic and magnetostatic potentials and fields
  - Charge density
  - Particle tracks, beam parameters and profiles
    - Momenta, energy, TOF, current etc





- **Allows evaluation of**
  - Target erosion profile
  - Target utilization
  - Deposition profile
  - Power deposition and thermal load
  - Losses to walls and structure

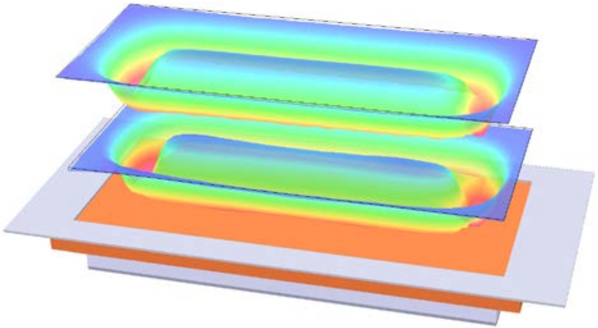


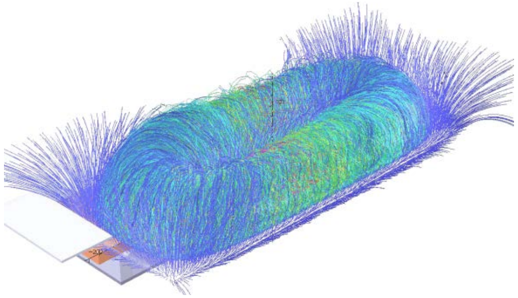


Magnetron simulation
sample results comparison

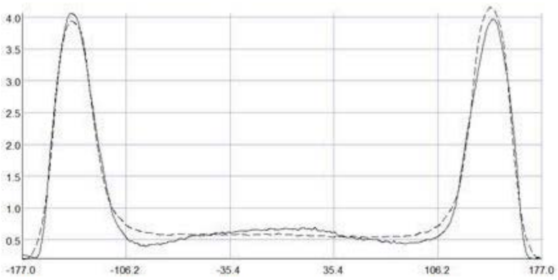
- **Validation against several different magnetron designs**
  - Teer Coatings Ltd.
  - Utilization
    - Simulated 35.73%
    - Measured 35.30%

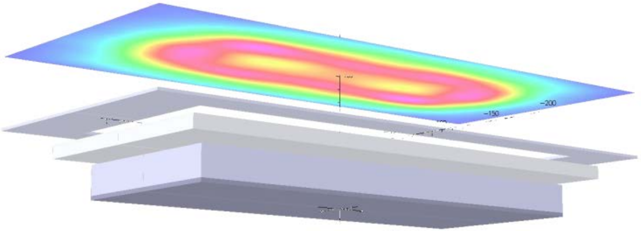
Plasma electrons above the target





Erosion profile – measured and simulated



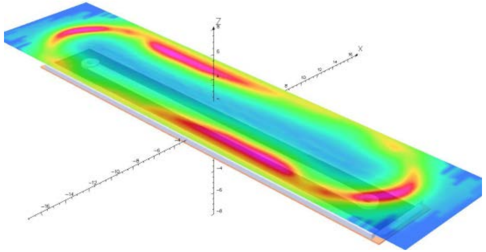


Sputtered particle distribution at the substrate

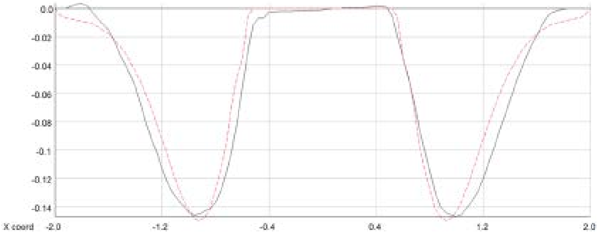
Magnetron simulation
sample results comparison

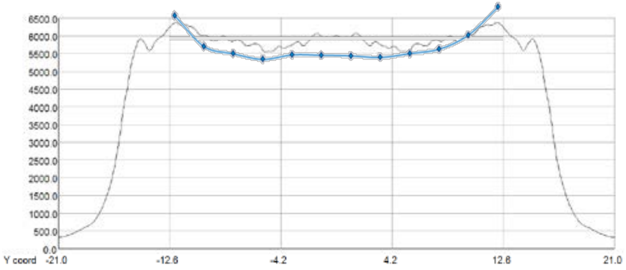
- **Validation against several different magnetron designs**
  - Colorado Concept Coatings LLC.
  - Utilization
    - Simulated 25.90%
    - Measured 26.44%

Ar ion beam profile at the substrate

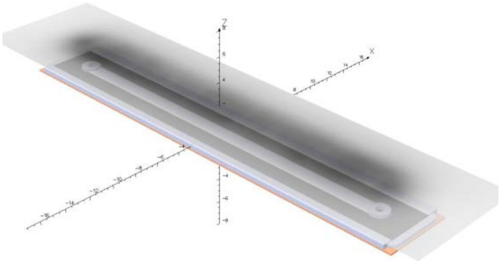


Erosion profile – measured and simulated



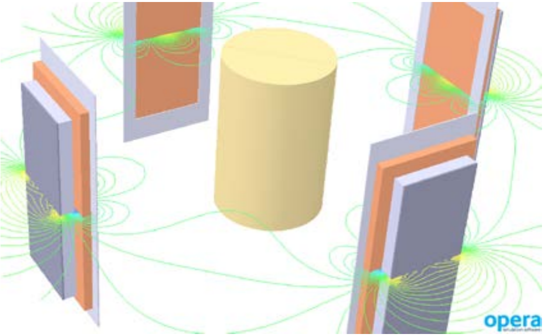


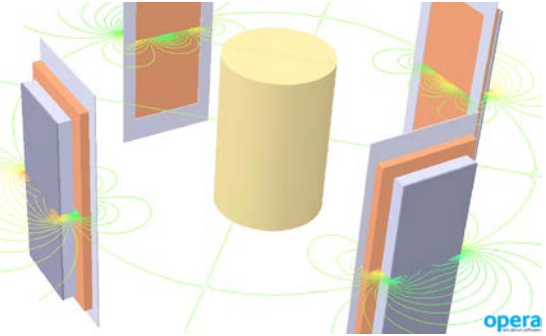
Sputtered particle distribution at the substrate

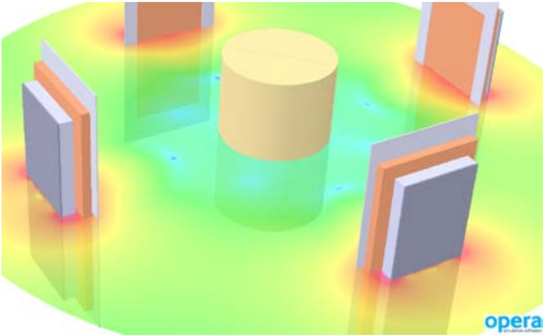


Magnetron coater simulation

- **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