Three-Dimensional Full-Wave Optical Simulations with OPUS 3-D

Martin Loeser

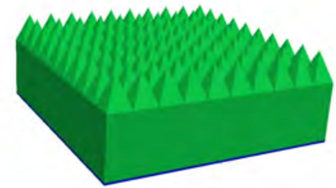
Zurich University of Applied Sciences

Table of Contents

Introduction & Motivation

Design of LEDs with Textured Surfaces

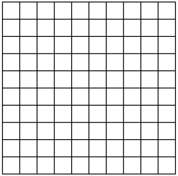
- Goal: model light propagation inside optically large structures such as LEDs or solar cells
- Challenge: modern devices are large in size and feature textured surfaces
- New full-wave approach: the Ultra-Weak Variational Formulation (UWVF)



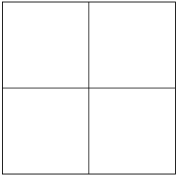
Three-dimensional LED structure with textured surface and bottom mirror.

Main Features of the Ultra-Weak Variational Formulation

- Discontinuous Galerkin Finite Element approach with plane wave base functions
- Discretized version: $(D - C)\mathbf{x} = \mathbf{b}$
- High accuracy on coarse meshes
- Memory consumption decreased by up to 70% $\longleftrightarrow$ standard FEM
- System matrix tends to show ill-conditioning, active regions are complicated to treat



FEM: $\lambda/10 \times \lambda/10$



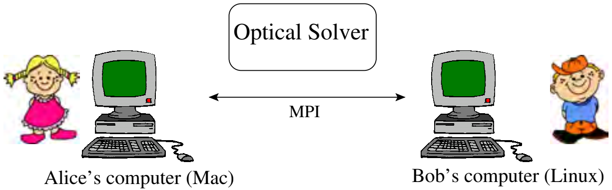
UWVF: $2\lambda \times 2\lambda$

OPUS 3-D

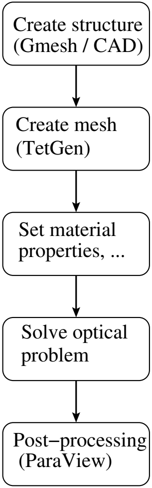
Optical Parallel Ultra-Weak Solver

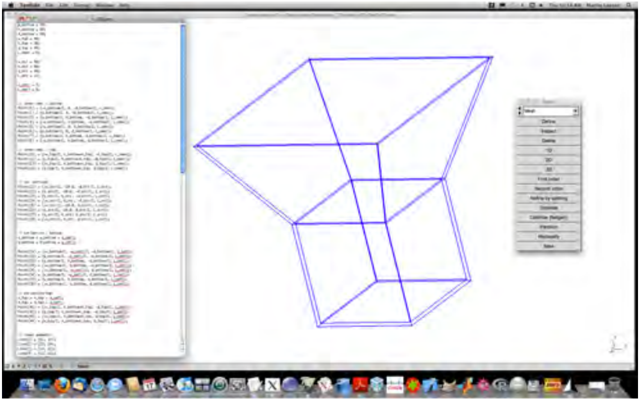
Basic Features of OPUS 3-D

- Maxwell's equations are solved on 3-D domains
- Ultra-Weak Variational Formulation implemented in C++
- Applicable to nearly arbitrary geometries
- Unstructured meshes → no need to use tensor meshes
- Dynamic selection of base functions → numerically stable
- Parallelization using MPI → suitable for shared and distributed memory machines



Simulation Flow Diagram



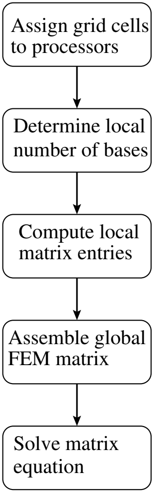


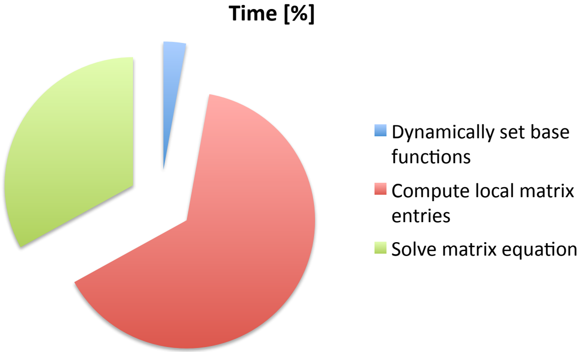
Gmsh as front end for structure generation and meshing (2-D & 3-D).

Example: Treatment of a Complex CAD Structure

Simulation of the institute logo—device structure imported from CAD tool *Catia*. No need to use tensor meshes.

Computational Tasks

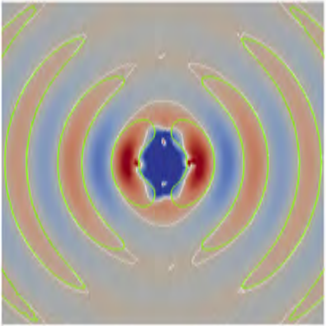


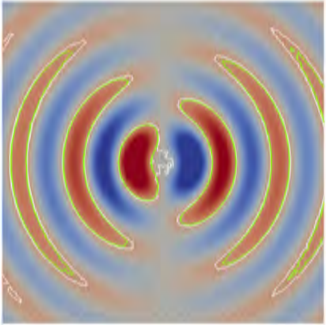


More than 70% of the computation time is dedicated to entirely independent tasks → efficient parallelization.

3-D Model Problems

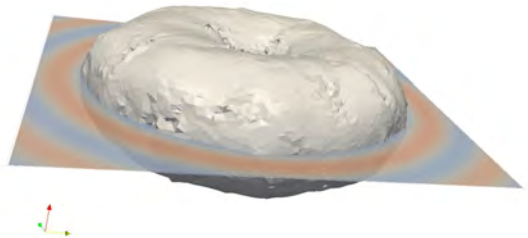
Dipole Radiating into Free Space (I)





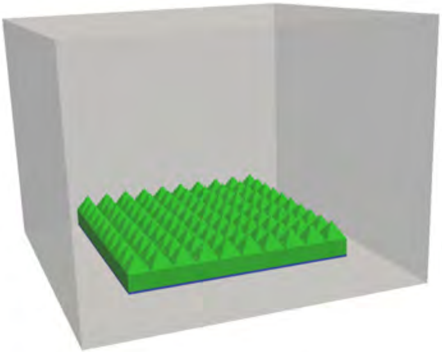
Left picture: isoclines of E_x field component – green is the analytical solution, gray is the OPUS 3D result (in V/m).
Right picture: isoclines of H_z field component – green is the analytical solution, gray is the OPUS 3D result (in A/m).

Dipole Radiating into Free Space (II)



The donut-shaped emission beam calculated with OPUS 3D.
Simulation domain: $10\,\lambda \times 10\,\lambda \times 10\,\lambda$.
Memory requirements: $17\,\mathrm{GByte}$ for highest accuracy.

LED Model Problem—Optical Characteristics

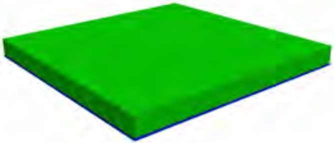


Three-dimensional LED structure with textured surface (green) and surrounding air (gray).
Device size: 10 µm × 10 µm × 1.5 µm

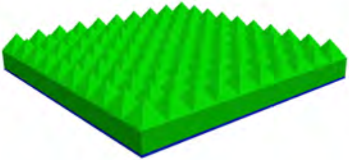
Simulator helps to answer the following questions

- Radiated power?
- Shape of the emission beam?
- Impact of surface structure?

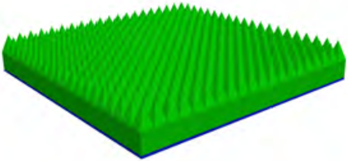
Comparison of Three Different Device Designs



flat

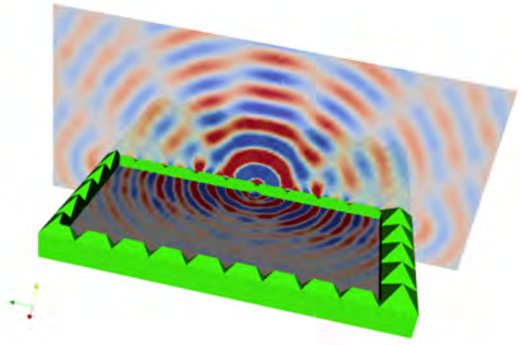


100-pyramid texture



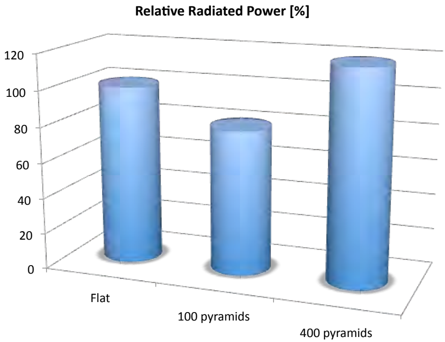
400-pyramid texture

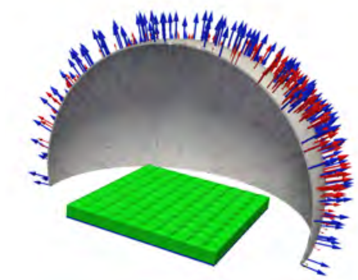
Solution of Maxwell's Equations—E-field Distribution



- Dipole source inside LED
- Plot shows E_x component
- Domain Size: $25\lambda \times 25\lambda \times 4\lambda$
- Required Memory: $8\,\mathrm{GB}$
- Computation Time: $7\,\mathrm{min}$ on 7 processors

Impact of Surface Texture on Radiated Power

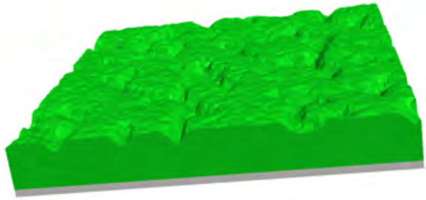


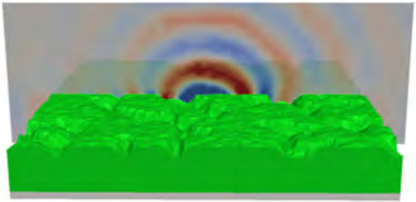


Radiated power as surface integral: $P = \oint \mathbf{S}\, d\mathbf{A}$. First texture decreases radiated power by 20%, second texture increases radiated power by 18%.

Simulation of Realistic Devices

Simulation model—surface structure was derived from AFM measurements.





Summary and Outlook

Summary

- OPUS 3-D solves Maxwell's equations in 3-D
- Lossy materials and PEC have been incorporated
- Qualitative and quantitative evaluation of surface textures possible

Future Activities

- Benchmark with measured data
- Further increase computational efficiency $\longrightarrow$ information reduction schemes
- Transition to larger and more realistic devices

Thank you for your attention!