Simon Cox (University of Southampton)
Engineering Workflows (= ‘Scripts’)

• Scenario: Design optimisation
  ➢ Model device, discretize, solve, postprocess, optimise

• Scripting approach
  ➢ Flexibility & High-level functionality
  ➢ Quick application development
  ➢ Extend user’s existing PSE e.g. Matlab, Python, ...
  ➢ … is our execution/ enactment engine too

• Favourite things to do
  ➢ Create, Retrieve, Cut ‘n’ Shut (Re-use anything and everything)
  ➢ Configure, Execute, Monitor (Bring Grid to user)
  ➢ Share, Steer, Dynamically modify (Semantic support)
Photoonic Crystal - Optimisation

Location, size & density of holes determine the optical bandgap.

The aim of this design optimisation process is to find a configuration which maximises this bandgap and minimizes energy loss.

User: Molinari
CAD Model A
Parameter 1: Rad
Parameter 2: Pos
Optimise BGap
Computed X Iter

Energy Bandgap

Grid-Enabled Scripting Environment

• Motivations:
  - Flexible, transparent access to computational resources
  - Easy to use for engineers (and in widespread use)

• Our Approach
  - Matlab chosen as the hosting environment
    - Extend the user’s existing PSE
    - High-level functionality
    - Quick application development
    - … is our execution=enactment engine too
  - Computational resources exposed in the form of Matlab functions
    - Job submission to Globus server using Java Cog
    - Job submission to Condor pool via Web services interface
  - Integration of CAD, Mesh generation, and Fluent solver via the use of intermediate data format, often standard-based, or package-neutral
  - Hybrid search strategies to make the best use of different search methods

• Can also use Python, Jython, etc.