Optimization of the Temporal Shape of Laser Pulses for Ablation

Company: Institut nationale d’optique

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Industry participant: Alain Cournoyer

Outline

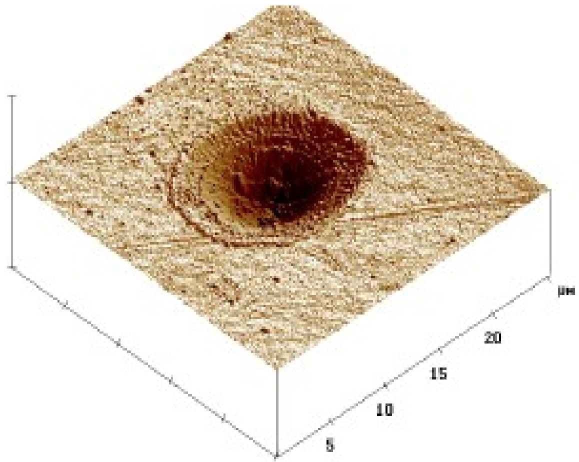
- Problem setup
- Modeling/Computational strategy
  - Physical model
  - Numerical scheme for solving PDE
  - Optimization strategy
- Results
- Outcomes for INO
- Conclusion and perspective

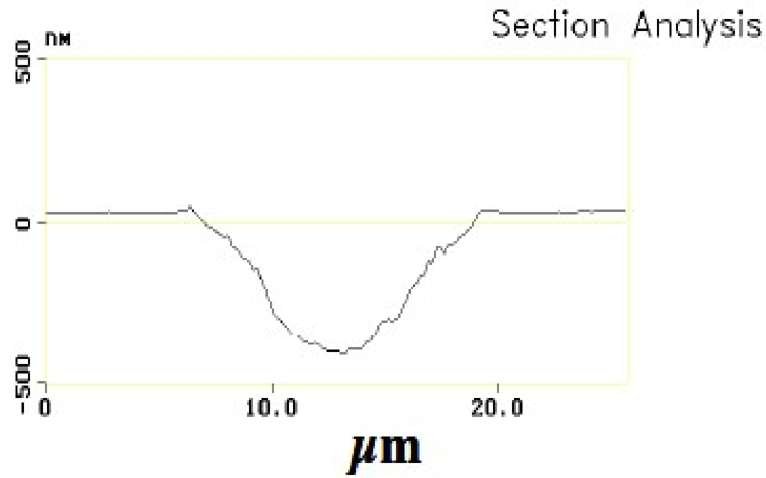
Problem Setup

- Problem: Find temporal shape of laser pulse optimizing ablation.

- Function to optimize

  "Efficiency" = J = depth/(energy of pulse)

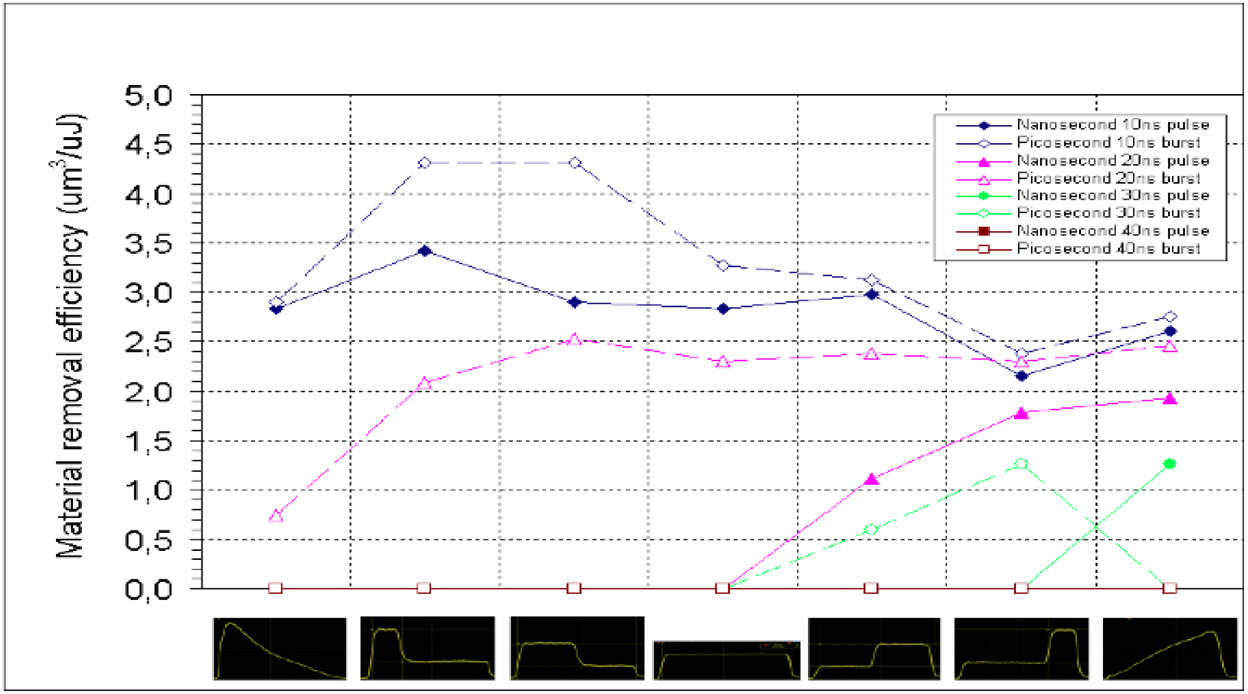




Needs:

- Computational strategy
- Physical parameter values
- Ultimately: Laboratory experiments

Current Experiments



- Typical results show :
  - Si : about 1/2 of estimated max efficiency
  - Al and steel : about 1/6 of estimated max efficiency

Some Physics

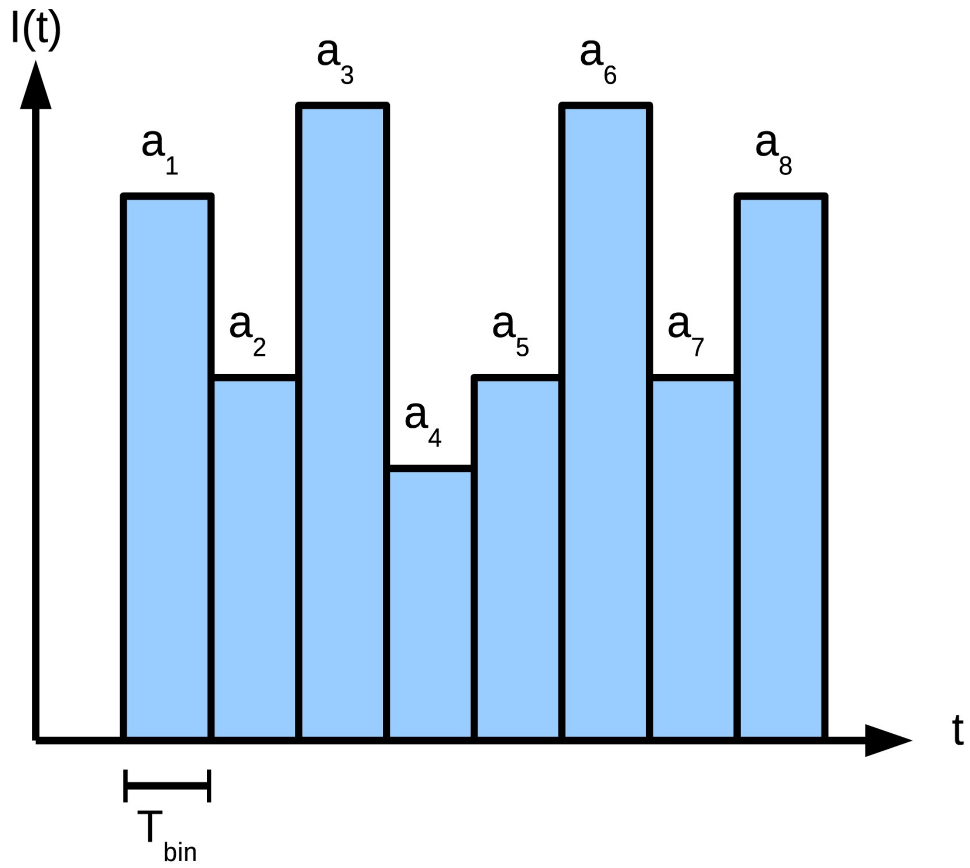
- Expect different pulse shapes for different materials
  - Important physical parameters:
    - Optical absorption coefficient
      - Not available for the range of required values
      - For silicon above melting temp (~1600 K), but need value up to vaporization temp (~3500 K)
    - Latent heat of vaporization
- This week: focused on silicon

Temporal Pulse Shape

$$I(t) = \sum_{i=1}^{256} a_i \chi_{\omega_i}(t)$$

$$T_{bin} = |\omega_i| \quad (\sim 2.5 \text{ ns})$$

$$E_p(J/m^2) = T_{bin} \sum_{i=1}^{256} a_i$$



Computational Strategy

- 1. Solve PDE for heat transfer to obtain depth of ablated material
- 2. Use depth from (1) to obtain value for objective function for optimization
  - We have explored two different optimization methods
    - Simulated annealing (logarithmic cooling schedule)
    - “Multistart optimization” to find global minima + ensemble of local minima
  - Tested on sample problems

Physical Model

- Heat transfer equation (BVP)

$$\frac{\partial H}{\partial t}+u_{vap}\frac{\partial H}{\partial x}=\frac{\partial}{\partial x}k(T)\frac{\partial T}{\partial x}+\frac{\partial I}{\partial x}$$

$$H=\rho C_p T$$

- Boundary conditions

$$-k(T)\frac{\partial T}{\partial x}|_{x=0}=u_{vap}H_{vap}\rho \qquad T(-L,t)=T_{room}$$

- Initial condition

$$T(x,0)=T_{room}$$

Physical Model

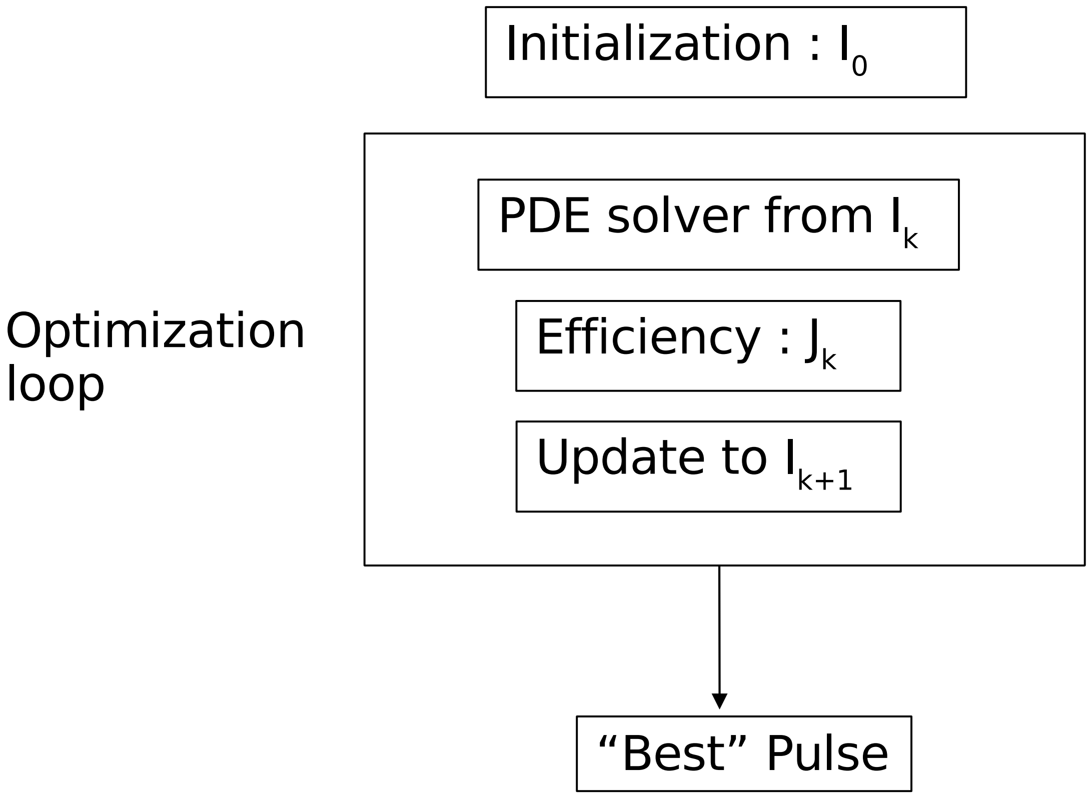
- Laser beam intensity

$$\frac{\partial I}{\partial x}(x,t)=\alpha(T)I(x,t)$$

- Vaporization velocity
  - Moving Boundary
  - Depends on surface temperature
  - Given by Hertz-Knudsen equation
  - Allows to compute depth of ablation

$$\Delta z=\int_0^{t_{final}} u_{vap}(s)ds$$

General Algorithm



Numerics

- Numerical Solver ((too) simple at this stage)
  - Semi-implicit scheme
  - Stability condition from convection term
  - Necessitates linear system computation :-(

$$\underline{\underline{A}}(dt^n)\underline{T}^{n+1}=\underline{\underline{B}}(dt^n)\underline{T}^n+\underline{F}(dt^n, BC, source)$$

  - Careful computation of boundary conditions
- More specific solver for Stefan like problems to be implemented

Simulated Annealing

- Simplest Monte Carlo type optimization
- Easy to implement
- Normalization of pulse parameters to satisfy

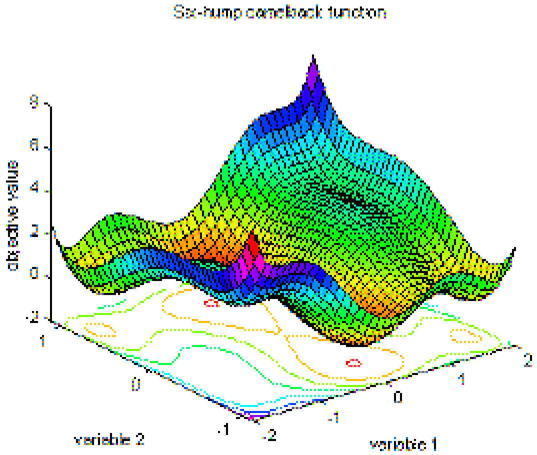
$$E_p(J/m^2) = T_{bin} \sum_{i=1}^{256} a_i$$

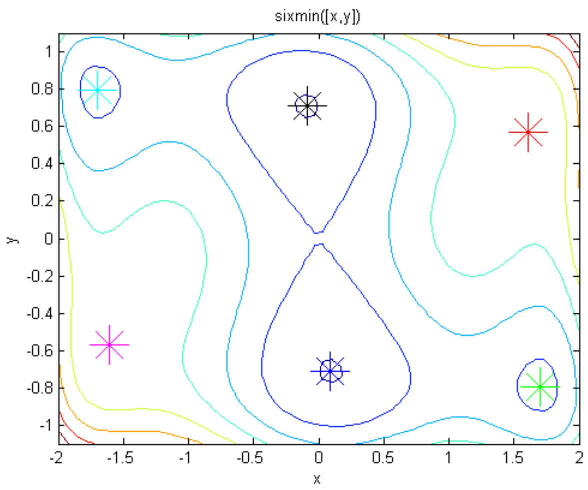
MultiStart Method

- MultiStart explores energy landscape while simultaneously finding both local and global minima
- MultiStart has two phases – global phase and local phase
- Global phase: Performs scatter search to cover the domain
- Local phase: Performs gradients to converge to local minimum

Global Optimization Toolbox (Matlab)

Simple Test Function: Six Camelback Hump Problem





- Properties of six camelback hump problem**:** (1) six local minima
- The MultiStart method finds all minima

Challenges with Using MultiStart on our Industrial Problem

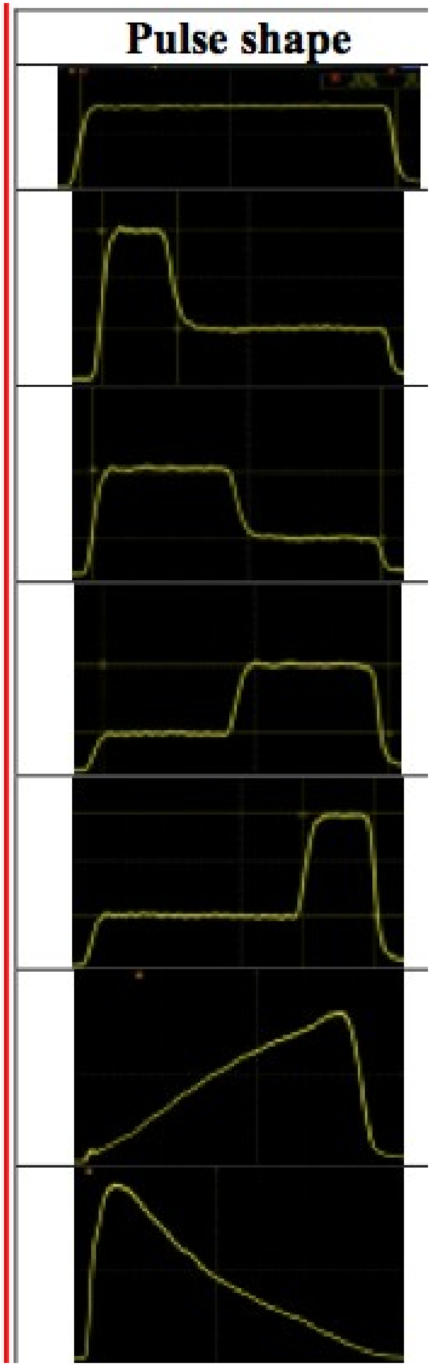
- Determining which local minima are relevant but return all local minima
- Because method uses gradient, may be intractable for large problems
- Numerical instability in calculations may occur unless preconditioner is used for Hessian

Issues

- Get accurate PDE code to work with physical values of parameters
- Uncertainty in physical parameter values and physical model (!) necessitates caution with answers from optimization
  - E.g. Importance of local minima to explore different parts of solution space (i.e., find different pulses with different qualitative features)

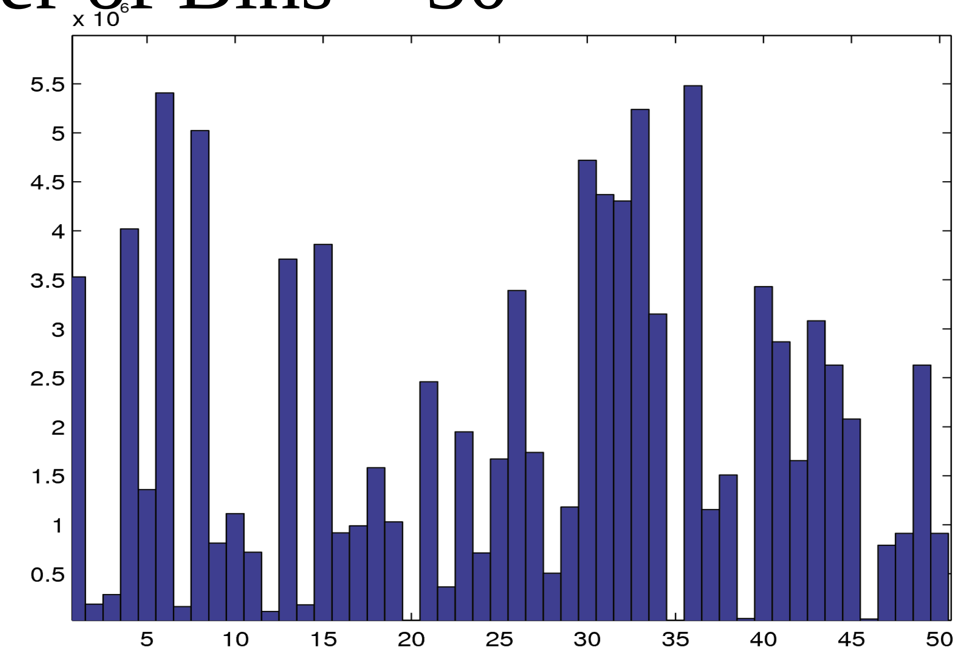
Pulse Shapes

- Experiments suggested left-heavy ones for Si, though only small number of shapes (see figure on right) were checked
- Also obtain left-heavy pulses with optimization...



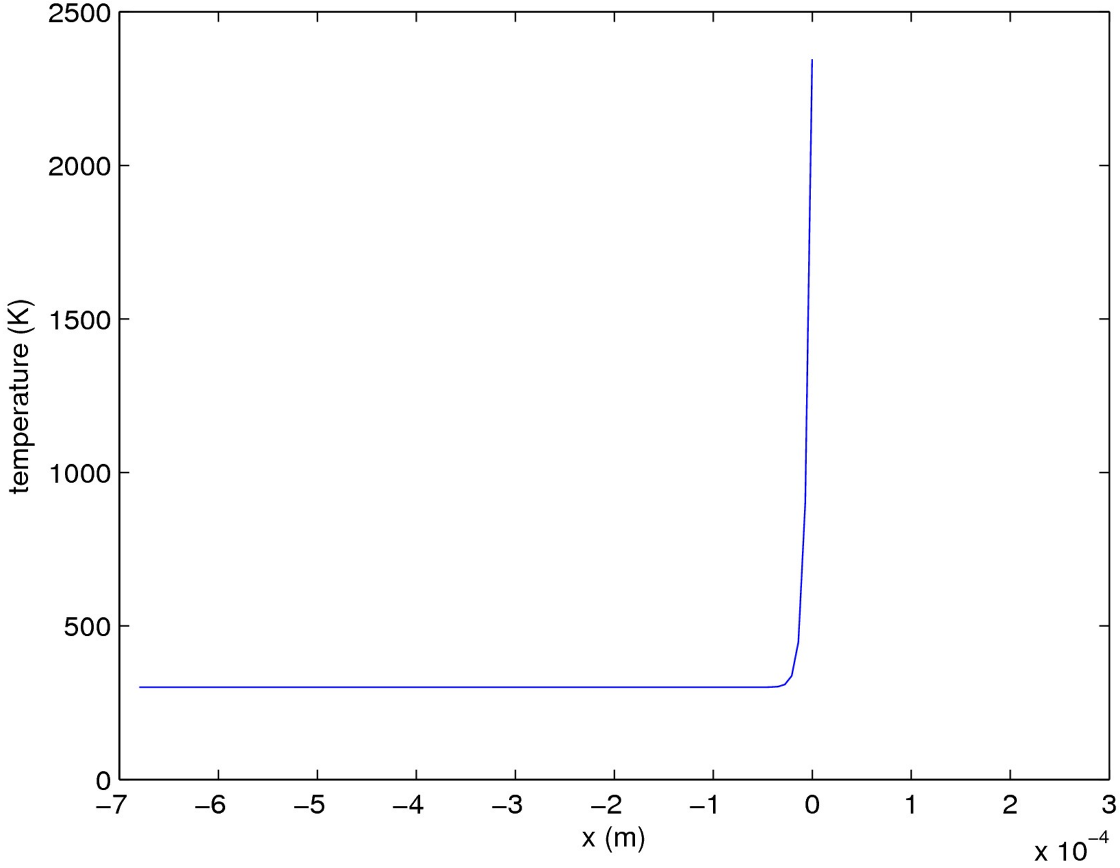
Numerics

- From physical experiments
- Number of Bins = 50

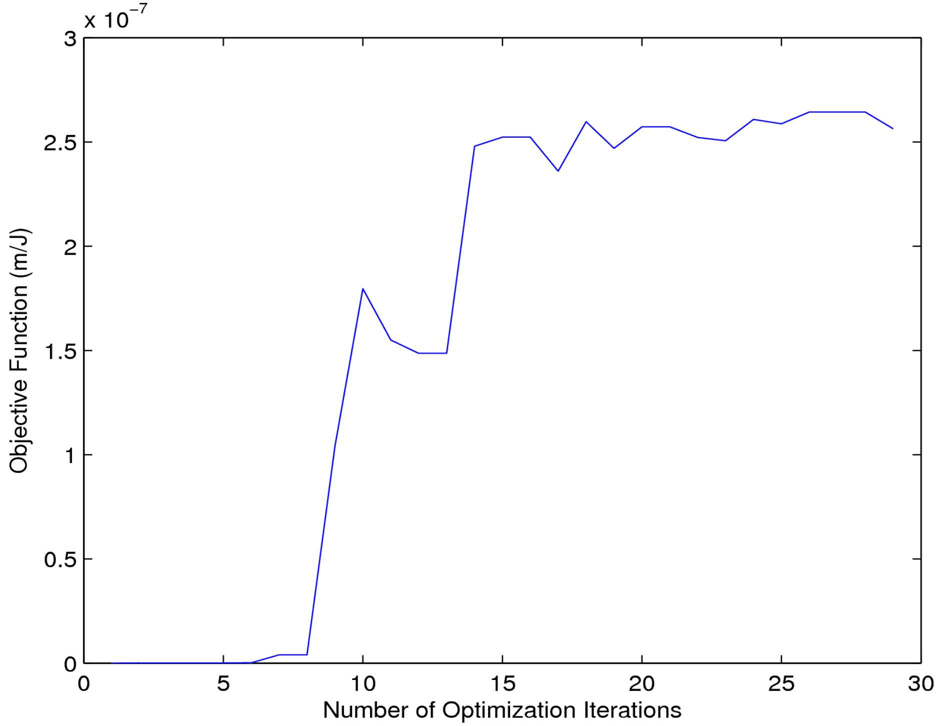


- Results very sensitive to physical data, in particular α

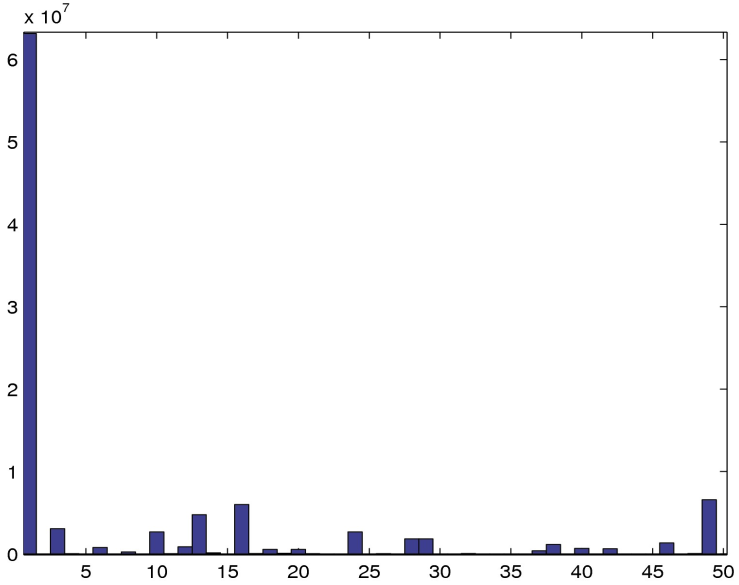
Temperature curve

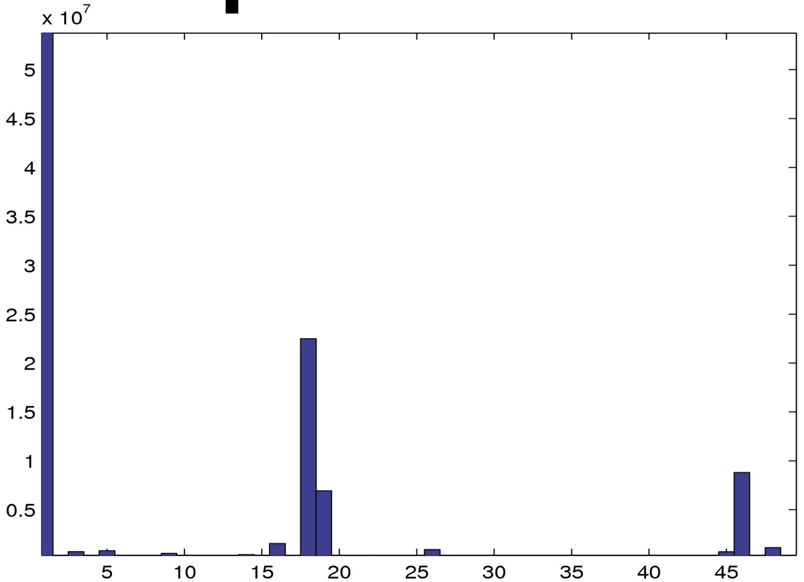


Optimization curve based on S.A.



Pulse shape


x 10^7
6
5
4
3
2
1
0
5 10 15 20 25 30 35 40 45 50


x 10^7
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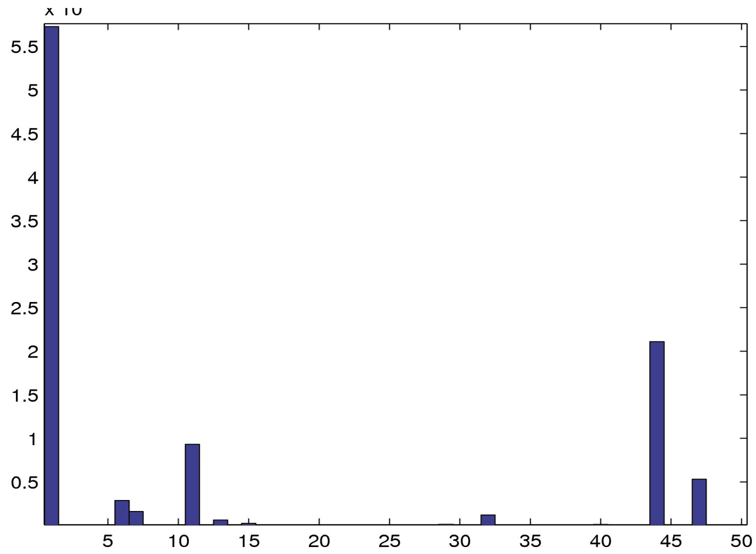
5.5
5
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2
1.5
1
0.5
5 10 15 20 25 30 35 40 45 50

The Importance of Being Local

- Need to find ensembles of local minima
- Gives qualitatively different pulses to use as inputs in experiments
- A local minimum could become global with changes in physical parameters, models, etc (all of which are rather uncertain)

Outcomes for Company

- Preliminary Matlab code, including PDE simulator and two optimization methods (simulated annealing for global optimum and ‘multistart’ for local optima)
- Outcomes of optimization could suggest experiments with specific pulse shapes for silicon
- Few percent of efficiency improvement can result in monetary benefits

Conclusion and perspectives

- Improvement of the numerical code/model
- Optimization on multipulses laser ablation (repetition rate, scanning speed,...)
- Other useful objective functions
- Test result experimentally
- Multi-D