VERIFICATION AND VALIDATION: SOME EXPERIENCE FROM COMPUTATIONAL PRACTICE

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Outline

Outline

Determinism

"Given for one instant an intelligence which could comprehend all the forces by which nature is animated and the respective situation of the beings who composed it — an intelligence sufficiently vast to submit these data to analysis — it would embrace in the same formula the movements of the greatest bodies of the universe and of the lightest atom; for it, nothing would be uncertain and the future, as the past, would be present to its eyes."

Laplace, 1776

Determinism

Such an intelligence has yet to be found!

$\Rightarrow$ Create theories with simplifying assumptions to *approximately* predict the past, present, and future.

What is a model

A representation of a phenomenon using existing physical laws and existing paradigms.

However,
physical laws are derived using simplifying assumptions.
(Example: Newton's laws.)

Simulations

Simulations are used to predict the model behavior to given sets of inputs/parameters.

Even if simulation results match the measurements, simulations are not exact predictors of reality.

Simulations

There are always *inaccuracies* between the simulation results and the reality because of:

- the limits and assumptions of the theory made to derive it
- the numerical method limits
- the simplification of the problem (for example, geometry or boundary conditions simplifications)
- variability and uncertainty of model parameters

Outline

What is meant by verification

Numerical *verification* — be certain the numerical method works correctly.

"Solving the equations right"

(*Roache*, Verification and Validation in Computational Science and Engineering, Hermosa Publishers 1998.)

Verification practice

Practice: verification is done independently of the model. It is a way of making sure the numerical method works on benchmark cases.

- Just testing, not verification?
- What about the code (program) of the model?

Outline

What is meant by validation

- Roache's (1998) definition:

  "Solving the right equations"

- Our definition: "A method to attain a pre-defined level of accuracy for a model and its simulation results."

$\Rightarrow$ Reach a certain confidence in the model's correctness.

Validation objectives

- assess model performance objectively
- account for numerical method limits, model parameters variability and uncertainty
- evaluate the results of a simulation without human bias and interpretation

The goal of validation

Validation is not . . .

- *Model tuning*: model tuning does not imply having a model validated. However, an updated model can be validated.
- *A substitute for user's training*. It is meant to help him get a better model and make better decisions.

The Goal

- Use numerical model with confidence to predict response with few or **no** experiments.

Outline

Standard boundary value problems

- we look for the solution u of a given system of differential equations on a domain $D \subset R^n$

$$Au = f \quad \text{in} \quad D$$

- u should satisfy some set of conditions on the boundary ∂D of D

$$Bu = g \quad \text{on} \quad \partial D$$

Examples of standard boundary value problems

Examples:

- Dirichlet problem for the Poisson equation

$$-\Delta u = f \quad \text{in} \quad \Omega$$

$$u = g \quad \text{on} \quad \partial\Omega$$

- initial-boundary value problem for the heat transfer equation on $\Omega \times [0, T]$

Outline

Unknown-boundary value problems

- domain D is not known or completely specified
- examples: falling raindrop, Czochralski method of crystal growth, flow through porous media, diffusion of oxygen in a body tissue
- additional information required relating the solution u of the differential system to its domain of definition D

Unknown-boundary value problems

- additional boundary (or interface) conditions along the unknown part Γ of ∂D (or along the unknown interface $\Gamma \subset D$):

$$Cu = h \quad \text{on} \quad \Gamma$$

- solution of an unknown-boundary value problem is the pair $\{u, \Gamma\}$
- inherent nonlinearity of geometrical nature
- *free boundary problems*: stationary
- *moving boundary problems, MBPs*: evolution

Examples of unknown-boundary value problems

The Classical Two-Phase Stefan Problem

A model of a slab of "ice" melting from the left: Find the temperature $T(x,t)$, $0 \leq x \leq l$, $t > 0$, and interface location $Z(t)$, $t > 0$, such that the following are satisfied:

- partial differential equations

$$\frac{\partial T}{\partial t} = \alpha_L \frac{\partial^2 T}{\partial x^2} \quad \text{for} \quad 0 < x < Z(t), \;\; t > 0 \;\; (\textit{liquid region})$$

$$\frac{\partial T}{\partial t} = \alpha_S \frac{\partial^2 T}{\partial x^2} \quad \text{for} \quad Z(t) < x < l, \;\; t > 0 \;\; (\textit{solid region})$$

Examples of unknown-boundary value problems

- interface conditions

$$T(Z(t), t) = T_{\mathrm{m}}, \quad t > 0$$

$$\rho\lambda Z'(t) = -k_L \frac{\partial T}{\partial x}(Z(t)^-, t) + k_S \frac{\partial T}{\partial x}(Z(t)^+, t), \quad t > 0$$

- initial conditions

$$Z(0) = 0$$

$$T(x, 0) = T_{\mathrm{init}} < T_{\mathrm{m}}, \quad 0 \leq x \leq l$$

(the initial state is solid)

Examples of unknown-boundary value problems

- boundary conditions

$$T(0,t) = T_L > T_\mathrm{m}, \quad t > 0 \quad \text{(imposed temperature)}$$

$$-k_S \frac{\partial T}{\partial x}(l,t) = 0, \quad t > 0 \quad \text{(insulated boundary)}$$

Examples of unknown-boundary value problems

Analytical Solution to One-Phase Stefan Problem

$$\frac{\partial T}{\partial t} = \alpha_L \frac{\partial^2 T}{\partial x^2}, \ 0 < x < Z(t), \ t > 0 \ \textit{(liquid)}$$

$$T(Z(t), t) = T_\mathrm{m}, \quad t \geq 0$$

$$\rho\lambda Z'(t) = -k_L \frac{\partial T}{\partial x}(Z(t), t), \quad t > 0$$

$$Z(0) = 0 \quad \text{(material initially completely solid)}$$

$$T(0, t) = T_L > T_\mathrm{m}, \quad t > 0$$

Examples of unknown-boundary value problems

$$\mathrm{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-s^2} \mathrm{d}s, \quad St_\lambda = \frac{c_L(T_L - T_\mathrm{m})}{\lambda} \quad \textit{(Stefan Number)}$$

$$T(x,t) = T_L - (T_L - T_\mathrm{m}) \frac{\mathrm{erf}(\frac{x}{2\sqrt{\alpha_L t}})}{\mathrm{erf}(\omega)}, \quad Z(t) = 2\omega\sqrt{\alpha_L t}$$

$$\omega e^{\omega^2} \mathrm{erf}(\omega) = \frac{St_\lambda}{\sqrt{\pi}}$$

Mathematical Model of Laser Irradiation

- a sample of monocrystalline semiconductor (one-component material) irradiated by a laser pulse with energy density E
- one-dimensional treatment (due to the dimensions and symmetry of the sample)
- melting, evaporating, and resolidification of sample surface
- D - thickness of the sample
- $Z_0(t)$ - liquid/vapor interface, $Z(t)$ - solid/liquid interface
- evaporation into vacuum - only liquid and solid treated explicitly, vapor removed from the surface immediately
- $T(x,t)$ - temperature

Mathematical Model of Laser Irradiation - equations

$$\rho c_L \frac{\partial T_L}{\partial t} = \frac{\partial}{\partial x}\left(k_L \frac{\partial T_L}{\partial x}\right) + (1 - R(t))\alpha_L(x) I_0(t) \times$$

$$\times \exp\left(-\int_{Z_0(t)}^{x} \alpha_L(\eta)\mathrm{d}\eta\right), \quad x \in [Z_0(t), Z(t)], \ t > 0$$

$$\rho c_S \frac{\partial T_S}{\partial t} = \frac{\partial}{\partial x}\left(k_S \frac{\partial T_S}{\partial x}\right) + (1 - R(t))\alpha_S(x) I_0(t) \times$$

$$\times \exp\left(-\int_{Z_0(t)}^{Z(t)} \alpha_L(\eta)\mathrm{d}\eta - \int_{Z(t)}^{x} \alpha_S(\eta)\mathrm{d}\eta\right), \quad x \in [Z(t), D], \ t > 0$$

Mathematical Model of Laser Irradiation - fixed boundaries

Initial and boundary conditions

$$T(x,0) = T_0 = \text{const.}, \ x \in [0, D],$$

$$Z_0(0) = Z(0) = 0,$$

$$T(D,t) = T_0, \ t > 0$$

Mathematical Model of Laser Irradiation - interfaces

Solid/liquid interface

$$\rho\lambda_{\mathrm{m}}\frac{\mathrm{d}Z}{\mathrm{d}t} = k_S\left(\frac{\partial T_S}{\partial x}\right)_{x=Z(t)+} - k_L\left(\frac{\partial T_L}{\partial x}\right)_{x=Z(t)-},$$

$$\frac{\mathrm{d}Z}{\mathrm{d}t} = -C_1\exp\left(\frac{-Q}{k_{\mathrm{B}}T_Z}\right)\left\{1-\exp\left[-\frac{\lambda_{\mathrm{p}}}{k_{\mathrm{B}}}\left(\frac{1}{T_Z}-\frac{1}{T_{\mathrm{m}}}\right)\right]\right\}$$

Liquid/vapor interface

$$\rho\lambda_{\mathrm{v}}\frac{\mathrm{d}Z_0}{\mathrm{d}t} = k_L\left(\frac{\partial T_L}{\partial x}\right)_{x=Z_0(t)+} - \epsilon\sigma(T_{Z_0}^4 - T_{\mathrm{ext}}^4),$$

$$\frac{\mathrm{d}Z_0}{\mathrm{d}t} = \frac{C_2}{\rho}\sqrt{\frac{M}{2\pi R_{\mathrm{g}}}}\,T_{Z_0}^C\cdot 10^{-(A/T_{Z_0})+B}$$

Mathematical Model of Laser Irradiation - schematic

Set of equations for the temperature field $T(x,t)$, the phase interface position $Z(t)$, and the temperature $T_Z(t)$ at the interface:

$$\rho c_L \frac{\partial T_L}{\partial t} = \frac{\partial}{\partial x}\left(k_L \frac{\partial T_L}{\partial x}\right) + E_L(x,t), \quad x \in [0, Z(t)], \ t > 0,$$

$$\rho c_S \frac{\partial T_S}{\partial t} = \frac{\partial}{\partial x}\left(k_S \frac{\partial T_S}{\partial x}\right) + E_S(x,t), \quad x \in [Z(t), D], \ t > 0$$

Initial and boundary conditions:

$$T(x,0) = T_0 = \text{const.}, \ x \in [0, D], \quad Z(0) = 0,$$

$$\frac{\partial T}{\partial x}(0,t) = 0, \quad T(D,t) = T_0, \quad t > 0$$

Mathematical Model of Laser Irradiation - schematic

Conditions at the moving phase interface $x = Z(t)$, $t > 0$:

$$\rho\lambda\frac{\mathrm{d}Z}{\mathrm{d}t} = k_S\left(\frac{\partial T_S}{\partial x}\right)_{x=Z(t)+} - k_L\left(\frac{\partial T_L}{\partial x}\right)_{x=Z(t)-},$$

$$\frac{\mathrm{d}Z}{\mathrm{d}t} = F(T_Z(t)).$$

Outline

Computational solution of MBPs

1. Choose an *initial approximation* $\Gamma^{(0)}$ of the unknown boundary Γ and put $k = 0$.
2. Denote by $\Omega^{(k)}$ the solution domain corresponding to $\Gamma^{(k)}$. Compute the function $u^{(k)}$ as the solution of the *standard boundary value problem*

$$Au^{(k)} = f \quad \text{in } \Omega^{(k)},$$

$$Bu^{(k)} = g \quad \text{on } \partial\Omega^{(k)}.$$

Computational solution of MBPs

3. Use the computed $u^{(k)}$ to find a *new position* $\tilde{\Gamma}$ of the *unknown boundary* in such a way that the interface condition(s) are satisfied on *this* $\tilde{\Gamma}$:

$$Cu^{(k)} = h \quad \text{on } \tilde{\Gamma}.$$

   Then put $k = k + 1$, $\Gamma^{(k)} = \tilde{\Gamma}$.

4. Compare $\Gamma^{(k)}$ with $\Gamma^{(k-1)}$ and if they differ more than a user supplied tolerance allows go back to Step 2. Otherwise, end the iteration and take $u^{(k)}, \Gamma^{(k)}$ for the final approximate solution.

- *successive approximation method* (trial and error)

Computational solution of MBPs

- real computations: discrete analogs of A–C are used
- *moving* boundary problems:
  - algorithm applied to the entire space-time domain
  - algorithm used to solve the free boundary problems obtained for each time level after time discretization
- the latter possibility seems to be preferable

Computational solution of MBPs

Three types of numerical methods

- *front-tracking methods*: special discretization formulas needed in the vicinity of the moving boundary
- *fixed-domain methods*: weak solutions, typical for more than one space dimension
- *front-fixing methods*: transformations of the independent variables

Computational solution of MBPs

Front-Fixing Methods

- **this is our approach**
- idea: to fix the moving boundary for the entire course of numerical solution
- the original MBP is transformed using a suitable transformation of space coordinates
- for the simple 1-D one-phase Stefan problem we may use

$$\xi = \frac{x}{Z(t)},$$

which fixes the moving boundary $x = Z(t)$ at $\xi = 1$ for all $t > 0$

Computational solution of MBPs

Front-Fixing Methods

- advantage: standard discretizations techniques can be used
- disadvantage: the partial differential equations achieve a complicated form; for the one-phase Stefan problem we arrive at

$$Z^2 \frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial \xi^2} + Z\xi \frac{\mathrm{d}Z}{\mathrm{d}t} \frac{\partial T}{\partial \xi}$$

- trial and error method used after front fixing (successive approximations)

Numerical algorithm

Resources

- approach proposed by R.M. Furzeland (*A Comparative Study of Numerical Methods for Moving Boundary Problems*. J. Inst. Maths Appl. 26:411–429, 1980)
- included into the well-known monograph by J. Crank (*Free and Moving Boundary Problems*. Oxford University Press, USA, 1987)
- feasibility documented by a series of numerical tests

Mathematical Model of Laser Irradiation - schematic

Set of equations for the temperature field $T(x,t)$, the phase interface position $Z(t)$, and the temperature $T_Z(t)$ at the interface:

$$\rho c_L \frac{\partial T_L}{\partial t} = \frac{\partial}{\partial x}\left(k_L \frac{\partial T_L}{\partial x}\right) + E_L(x,t), \quad x \in [0, Z(t)], \ t > 0,$$

$$\rho c_S \frac{\partial T_S}{\partial t} = \frac{\partial}{\partial x}\left(k_S \frac{\partial T_S}{\partial x}\right) + E_S(x,t), \quad x \in [Z(t), D], \ t > 0$$

Initial and boundary conditions:

$$T(x,0) = T_0 = \text{const.}, \ x \in [0, D], \quad Z(0) = 0,$$

$$\frac{\partial T}{\partial x}(0,t) = 0, \quad T(D,t) = T_0, \quad t > 0$$

Mathematical Model of Laser Irradiation - schematic

Conditions at the moving phase interface $x = Z(t)$, $t > 0$:

$$\rho\lambda\frac{\mathrm{d}Z}{\mathrm{d}t} = k_S\left(\frac{\partial T_S}{\partial x}\right)_{x=Z(t)+} - k_L\left(\frac{\partial T_L}{\partial x}\right)_{x=Z(t)-},$$

$$\frac{\mathrm{d}Z}{\mathrm{d}t} = F(T_Z(t)).$$

Numerical algorithm

Short description

- Landau transformation of both the phase intervals
- standard space and time discretization
- boundary conditions at the fixed ends $0, D$: standard procedure
- moving interface: one of the conditions processed in a standard way and included into the system of mesh equations
- moving interface: the other condition exploited in an iterative procedure to find the approximate value of $Z(t)$

Numerical algorithm

Result of the discretization

- some time level $t = t_n$
- notation: $\mathbf{u}$ - vector of approximate values of $T(x, t_n)$
- notation: s - approximation to the interface position $Z(t_n)$
- discrete boundary value problem to be solved:

$$\mathbf{A}(s)\mathbf{u} = \mathbf{b}(s),$$

$$s = f(\mathbf{u}, s)$$

- this system of nonlinear algebraic equations solved at each time step by iteration

Numerical algorithm

Iterative procedure

- choose s_0 and proceed for $k = 0, 1, \ldots$ as follows (until convergence):
- obtain $\mathbf{u}_k$ by solving the linear system

$$\mathbf{A}(s_k)\mathbf{u}_k = \mathbf{b}(s_k)$$

- then compute s_{k+1} from

$$s_{k+1} = f(\mathbf{u}_k, s_k)$$

- successive approximation method: *convergence*?

Outline

Verification of the Numerical Algorithm

- test example: classical two-phase Stefan problem (Neumann analytical solution)
- *convergence of the successive approximation method*: discretized Stefan condition

$$s = f(s)$$

- iterations $s_{k+1} = f(s_k)$ give $s_{k+2} \approx s_k$: oscillations, *no convergence*

Some theory of iterative methods

- $x = f(x)$, fixed point x^*; $\phi(x) \equiv x - f(x)$, zero x^*
- assumptions: x^* exists, f smooth enough
- successive approximation method (SAM)

Theorem. *If $|f'(x^*)| < 1$ then SAM is locally convergent. The rate of convergence is linear in general but if $f'(x^*) = 0$ it is quadratic at least.*

- what to do with SAM in case that $|f'(x^*)| \geq 1$ and the method does not converge?

Observations

- *Observation 1*: the same behavior when solving $s^2 = A$, $A > 0$, by successive approximations in the form $(f(s) = A/s)$

$$s_{k+1} = \frac{A}{s_k};$$

  remedy – Newton-Raphson method to solve $\psi(s) = 0$, $\psi(s) = s^2 - A$
- problem in our case: how to compute the values of $\psi' \rightarrow$ Newton's method inapplicable here

Observations

- *Observation 2*: Newton's method for solving $s^2 - A = 0$ has the form

$$s_{k+1} = \frac{1}{2}\left(s_k + \frac{A}{s_k}\right),$$

hence

$$s_{k+1} = \frac{1}{2}s_k + \frac{1}{2}f(s_k), \quad f(s) = \frac{A}{s}$$

- *relaxation*: rewrite the equation $s = f(s)$ to an equivalent equation $s = \alpha f(s) + (1-\alpha)s \equiv g_\alpha(s)$, $\alpha \in (0, 1]$
- optimum α found from the knowledge of the (approximate) value of $f'(s^*)$ and from the condition $g'_\alpha(s^*) = 0$:

$$\alpha = \frac{1}{1 - f'(s^*)}$$

Observations

- if $f'(s^*) \approx -1$ we obtain $\alpha \approx \frac{1}{2}$
- *Observation 3*: for $f(s) = A/s$ we have $s^* = \sqrt{A}$ and $f'(s^*) = -1 \rightarrow$ equivalence of the Newton-Raphson method and successive approximation method with underrelaxation in case of $\alpha = 1/2$

Outline

Remedy in our case

- put $F_\alpha(s) = \alpha f(s) + (1-\alpha)s \equiv g_\alpha(s)$, $\alpha \in (0,1]$
- the fixed points of f and F_α are identical
- try to choose α so that $F'_\alpha(s^*) = 0$ at a fixed point s^*
- optimum

$$\alpha = \frac{1}{1-D}, \quad \text{where} \quad D = f'(s^*)$$

- approximate D

A better iterative method

- assume we have a good initial approximation s_n of s^*
- compute $s_{n+1} = f(s_n)$, $s_{n+2} = f(s_{n+1})$
- put

$$D \approx D_n,$$

$$D_n = \frac{f(s_{n+1}) - f(s_n)}{s_{n+1} - s_n} = \frac{s_{n+2} - s_{n+1}}{s_{n+1} - s_n}$$

- use

$$\alpha_n = \frac{1}{1 - D_n}$$

- result:

$$\tilde{s}_{n+1} = \frac{s_n s_{n+2} - s_{n+1}^2}{s_{n+2} - 2s_{n+1} + s_n}$$

A better iterative method

- instead of solving $s = f(s)$ we solve $s = \tilde{F}(s)$ by the usual SAM, where

$$\tilde{F}(s) = \frac{sf(f(s)) - (f(s))^2}{f(f(s)) - 2f(s) + s}$$

Theorem. Let s^* be a fixed point of f such that $f'(s^*) \neq 0$, $f'(s^*) \neq 1$. Then the SAM for $\tilde{F}$ converges to s^* at least quadratically provided $|s^* - s_0|$ is sufficiently small.

- *the final method "well-known" in fact*:
  - Steffensen, J.F., Remarks on iteration, Skand. Aktuar. Tidskr. 16 (1933), 64–72
  - Willers, F.A., ZAMM 22 (1948), 125–126: "the method works always"

Verification – lesson learned

- the above approach (without relaxation) presented in Crank, J.: *Free and Moving Boundary Problems*, Oxford, Clarendon Press 1984
- suggested and tested (?) by Furzeland, R.M., A Comparative Study of Numerical Methods for Moving Boundary Problems, J. Inst. Maths Applics 26 (1980), 411–429
- test results published: "the scheme iterated until convergence (usually 2–3 iterations)"
- *do not trust even the reputable sources – do your own verification not only of your program but also of the method used*

Outline

Experimental situation

- GaSb samples (treated as one-component material) irradiated in vacuum ($< 10^{-10}$ Torr) by
  - ArF laser: $\lambda = 193\,\mathrm{nm}, 10\,\mathrm{ns}$ at FWMH
  - ruby laser: $\lambda = 694\,\mathrm{nm}, 80\,\mathrm{ns}$ at FWMH
- energy density varied in the range
  - ArF laser: 10–400 $\mathrm{mJ/cm^2}$
  - ruby laser: 50–1200 $\mathrm{mJ/cm^2}$
- changes in the optical parameters of the surface during pulse incidence monitored in situ by TRR using
  - for ArF laser - HeNe cw laser ($\lambda = 633\,\mathrm{nm}$)
  - for ruby laser - Nd:glass laser ($\lambda = 1.06\,\mu\mathrm{m}, 0.5\,\mathrm{ms}$)
- P. Přikryl, E. Gatskevich, G. Ivlev et al., Comput. Materials Sci. 17 (2000) 384

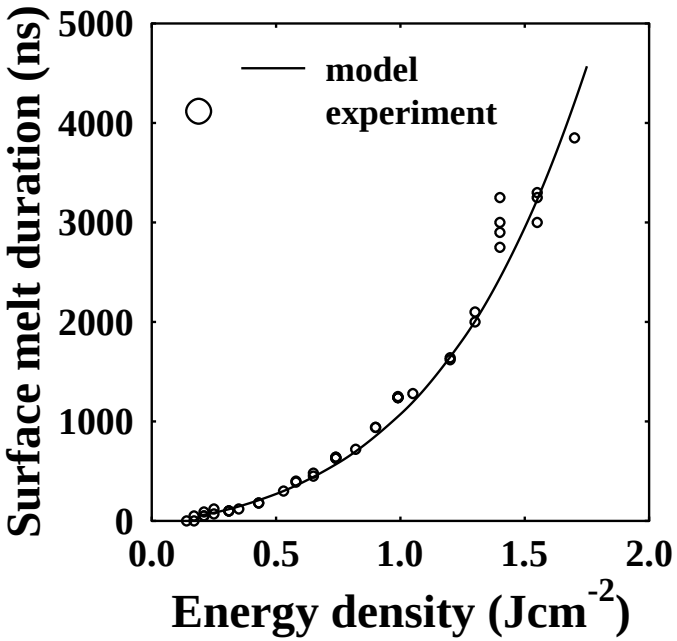
Computational simulations

- comparison of surface melt durations determined experimentally by TRR measurements and calculated by our model
  - a reasonable agreement for the ruby laser
  - no agreement for ArF laser

  (see figures)

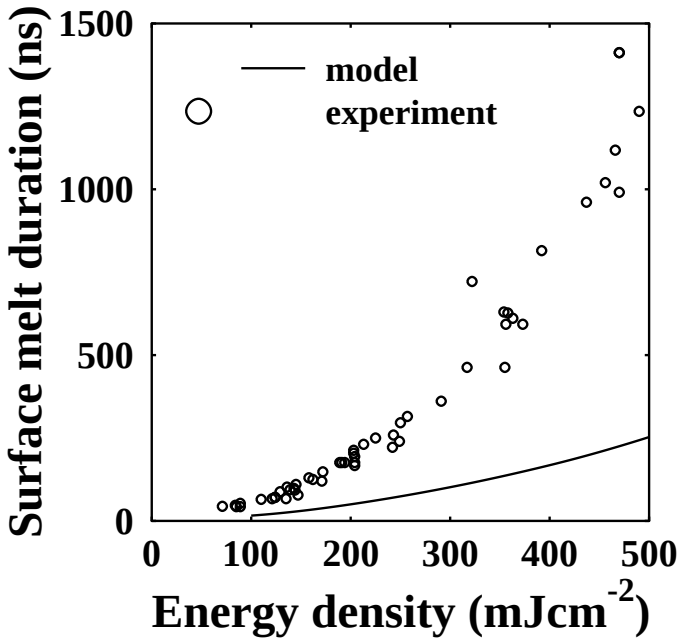
Comparison with the experimental results

Surface melt durations for ruby laser: computational model and experiment



Comparison with the experimental results

Surface melt durations for ArF laser: computational model and experiment

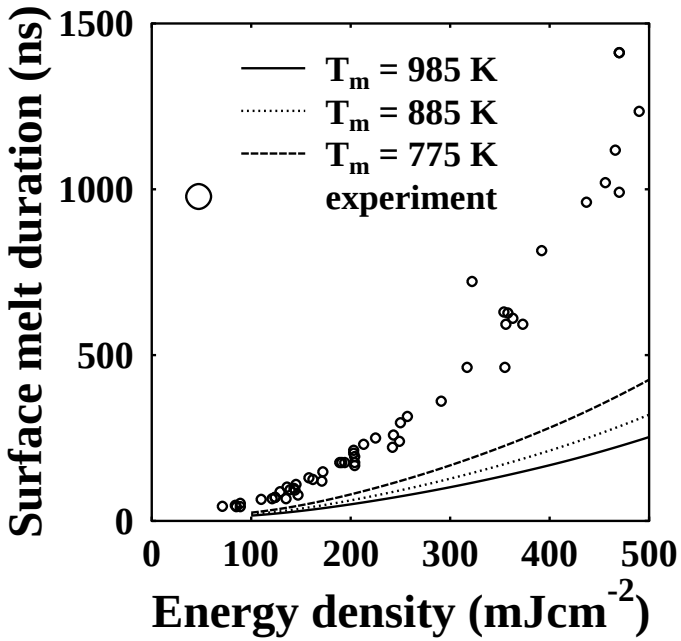


Possible explanation

- two hypothetical possibilities for explanation
  - decomposition of GaSb close to the melting point leading to significant changes in the melting temperature
  - substantial error in material parameters employed in the model (liquid reflectivity, thermal conductivity)
- test of the influence of all the parameters - see figures

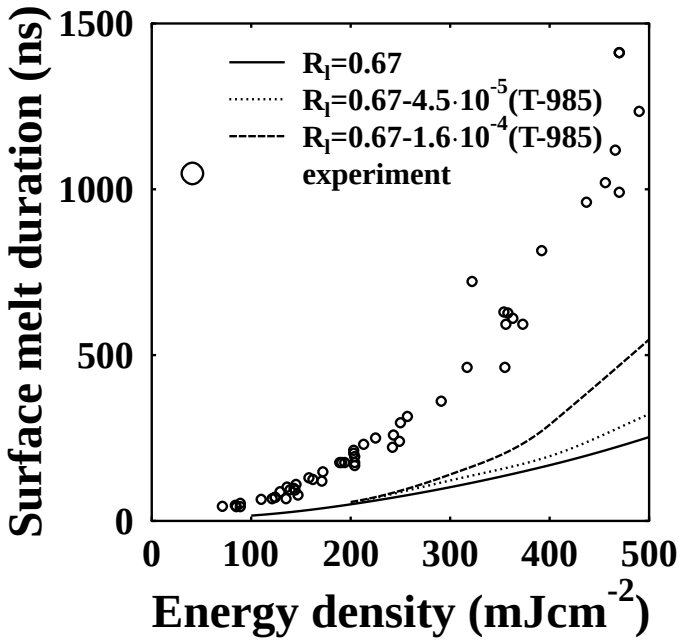
Comparison with the experimental results

Influence of the melting temperature on the surface melt duration (ArF laser)



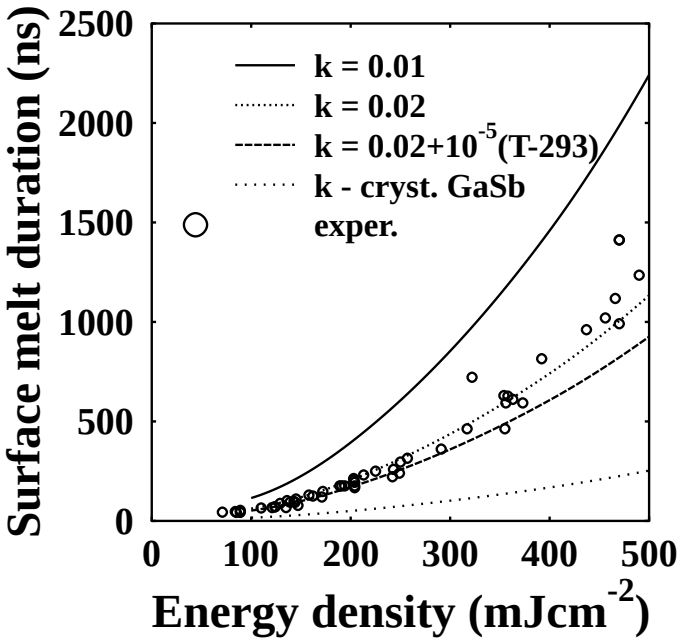
Comparison with the experimental results

Influence of the reflectivity of liquid on the surface melt duration (ArF laser)



Comparison with the experimental results

Influence of the thermal conductivity of solid on the surface melt duration (ArF laser)



Outline

Possible explanation – conclusion

change in thermal conductivity corresponding to amorphization of the surface layer

Amorphization – experimental validation I

- *low energy electron diffraction measurements* (LEED)
  - LEED pattern corresponded to a (1x1) structure below and at the melting threshold
  - further increase in the energy densities led to increase in the background and disappearance of diffraction spots
- *interpretation of the results:* amorphization of the irradiated layer indicated

Amorphization – experimental validation II

- *Auger electron spectroscopy* (AES)
  - smoothing of the structure in Ga and Sb peaks as compared to the state before irradiation
  - indicates increasing structural and chemical disorder
- *interpretation of the results:* correspond to supposed amorphization of the irradiated layer

Validation – lesson learned

- amorphization of GaSb samples after ArF laser irradiation confirmed by computational and experimental results
- do not think about the model only
- *model validation brought new information about the material used and the treatment applied*

Conclusions

- **verification** does not mean to verify the implementation of a trustworthy numerical method only
- the resources used should be subject to one's independent analysis
- **validation** can contribute not only to the quality of the computer model itself
- it can improve the knowledge of the system modeled as well