Strategies for handling different time-scales in CZ Silicon growth

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Introduction

We present numerical methods for simulating the transient growth interface shape.
Motivation:

- Time evolution of the interface is of interest in e.g. controlling the point defects [1]
- Time-averaged models (turbulence) in 2D are not always accurate enough [2]

The model tackles the following phenomena:

- Melt flow and convective heat transfer
  - ▷ Required time scale less than 1 s
- Evolution of growth interface
  - ▷ Required time scale ≈ 1 min
- Heater power control
  - ▷ Required time scale 10s of mins

⇒Multiscale model with respect to time is needed [3]

The basic idea is to use ideal algorithms for the whole range of timesteps
Methods are implemented into open source FEM software Elmer (`www.csc.fi/elmer`) [4]

Interface algorithms

The Stefan condition has to be satisfied on the phase change boundary:

$$\rho L \mathbf{v}\cdot\mathbf{n} = k_l \frac{\partial T_l}{\partial n} - k_s \frac{\partial T_s}{\partial n}, \qquad (1)$$

where ρ is the density of the solid, L is latent heat, $\mathbf{n}$ is the normal of the interface, T_s and T_l are the temperatures on the solid side and the liquid side of the interface, respectively, and k_s and k_l are the corresponding heat conductivities.

1) Steady state algorithm:
Set condition (1) with $\mathbf{v}\cdot\mathbf{n} = V$, solve thermal environment and find the isotherm $T = T_m$ (where V is the pull velocity)
   - robust & converges in a few iterations
   - suitable also for a transient simulation with time-averaged temperature (no latent heat)

2) Transient algorithm:
A derived form of Eq. (1) is used

$$\rho L v n_y - c\nabla^2 v = q_n \qquad (2)$$

where q_n is the normal heat flux (rhs of Eq. (1)), n_y is the y component of the normal vector, c is a small diffusion parameter, and the velocity v is defined to be y-directional.
Set $T = T_m$ as BC, solve thermal environment, evaluate q_n from Eq. (2), and solve for v. The displacement of the interface is then $u = (V - v)\,\mathrm{d}t$.
   - includes latent heat ⇒ correct inertia for growth interface evolution
   - heat flux computation sensitive to variations in temperature field (gradients)
   - may require relaxation to converge
   - similar approach often used, e.g. in [5]

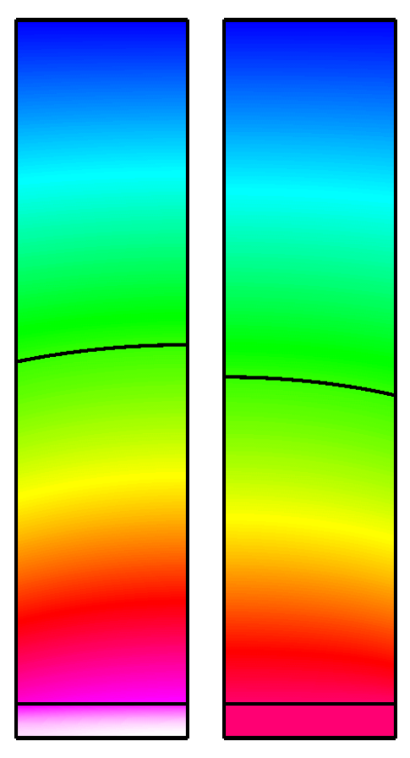
3) Hybrid algorithm:
Apply Robin boundary condition:

$$q_n = L\rho V + g(T_m - T) \qquad (3)$$

where $g = \frac{\rho\kappa}{dt V}$ and p is the fraction of the flux used in crystallisation.
T in Eq. (3) is treated implicitly in heat equation. After solving for temperature the flux disbalance is given by the penalty term in Eq. (3), and interface velocity is found from

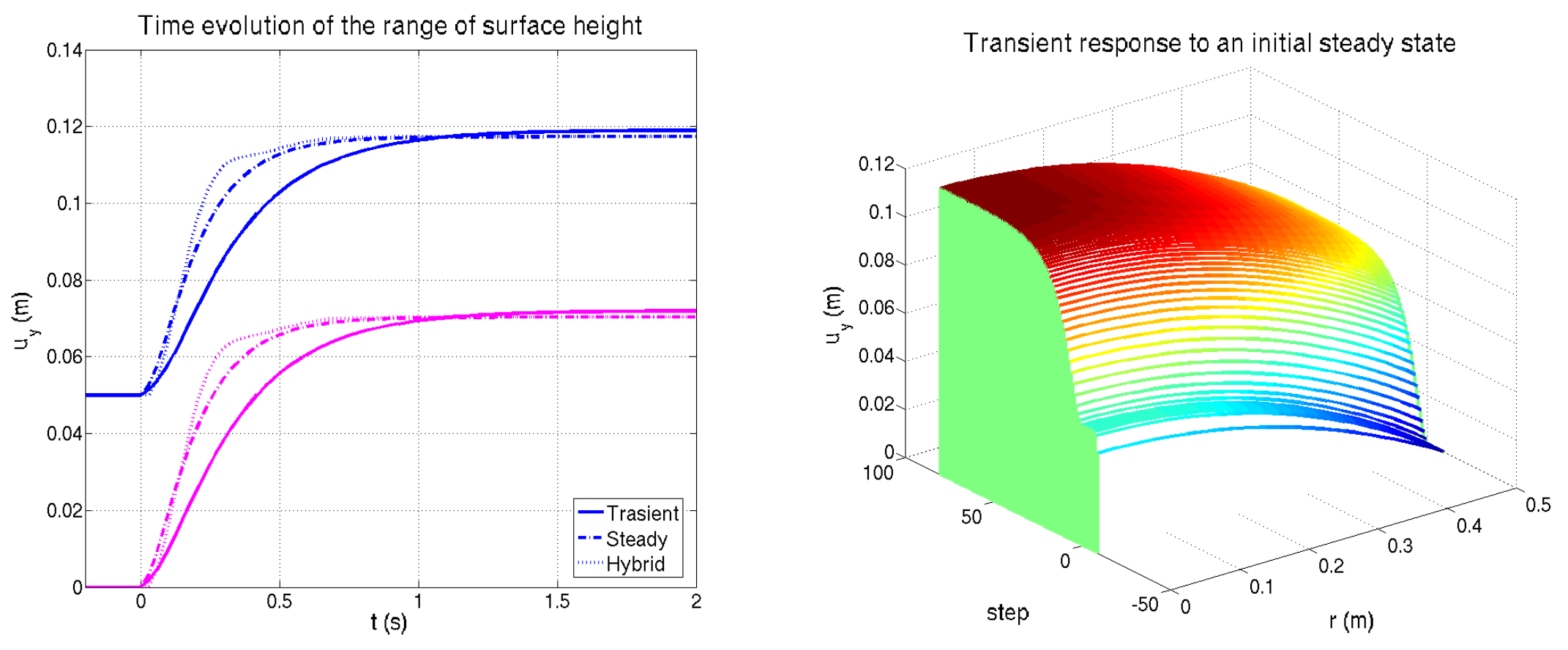
$$v = \frac{g}{\rho L}(T - T_m). \qquad (4)$$

   - constant flux condition combined with a physically meaningful penalty for temperature change
   - inertia of melting is accounted for
   - Changing BC type by tuning parameter p



Results in a cylindrical geometry; steady-state (top right) and a system heated from below without control applied (top left). The colors indicate the temperature distribution.

Time evolution of the end points (below left) and the whole interface (below right) are also shown.



Control algorithms

Control mechanisms are needed to keep the triple point stationary. Different algorithms for different regimes are possible.

1) Steady state temperature control:
Solve discretised heat equation in two parts, $A(T)\tau_0 = b$ and $A(T)\tau_1 = h$, where h is the controlled heat source. Assume that linear combination gives the full solution: $\tau = \tau_0 + \beta\tau_1$.
Require that $\tau|_{x_j} = T_m$ and thus the scaling factor to heater power is

$$\beta = \frac{T_m - \tau_0|_{x_j}}{\tau_1|_{x_j}}. \qquad (5)$$

The point x_j is the triple point. The method is closely related to that in [6].
   - exact control
   - combines well with steady state interface algorithm (flux condition for temperature)

2) Transient temperature control:
There is a relation between the change $\mathrm{d}h$ in heating power h and the change in temperature: $\frac{\mathrm{d}h}{h} = \gamma\frac{\mathrm{d}T}{T}$, where $\gamma \in [1, 4]$.
From the heat equation solution τ one may determine a scaling coefficient $\delta = \frac{T_m}{\tau|_{x_j}} - 1$ for temperature.
The heater power is adjusted by

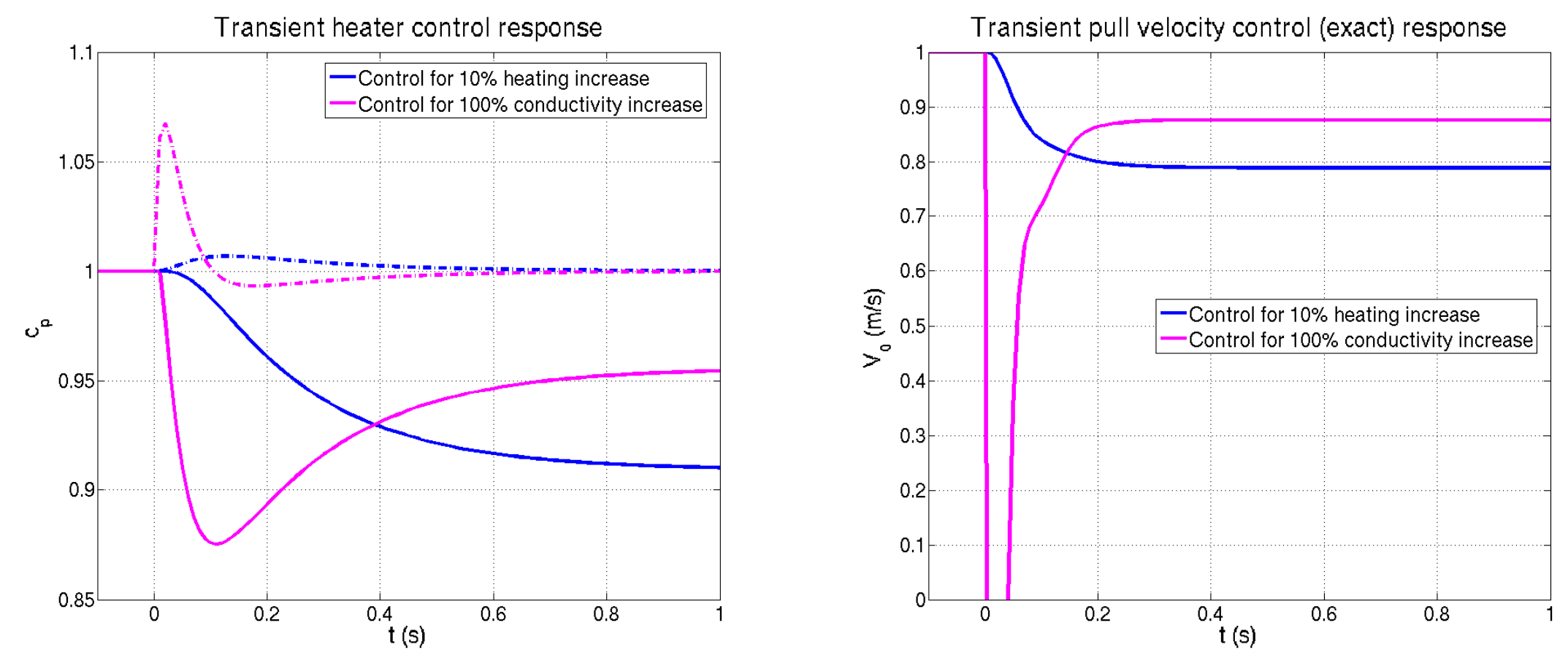
$$h' = (1 + \gamma\mu\delta)h \qquad (6)$$

and the temperature is updated by

$$\tau' = (1 + \mu\delta)\tau, \qquad (7)$$

μ is relaxation factor. Updating of temperature accelerates the propagation of heat from the heater to the vicinity of the interface.
   - combines well with averaged steady phase change algorithm (flux condition for temperature)

3) Transient velocity control:
Determine such pull velocity that the triple point position remains fixed
   - combines well with transient phase change algorithm (fixed temperature)



Results of control algorithms; heater response to disturbance in transient temperature control (left) and the adjusted pull velocity in transient velocity control.

Conclusions

- Methods for solving shape and evolution of the growth interface presented
- Models cover the whole range of time steps
- Growth interface algorithms and control strategies have been coupled
- The approach is proposed for CZ Si growth but is applicable also to other problems.

Future challenges

- Transition from one type of algorithm to another ⇒ different BC:s may create unphysical discontinuities
- A few model parameters that are hand-tuned
- Evaluation from steady state to true transient behavior still takes hundreds of timesteps (instead of thousands)
- Moving into the direction suggested in [7]

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