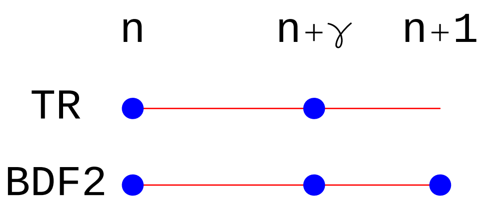
TRBDF2

R. E. Bank, W. M. Coughran, W. Fichtner, E. H. Grosse, D. J. Rose, and R. K. Smith, "Transient Simulation of Silicon Devices and Circuits," *IEEE Transactions on Computer-Aided Design*, **CAD-4**, 436–451, 1985.

M. J. Johnson and C. L. Gardner, "An Interface Method for Semiconductor Process Simulation," in *Semiconductors*, IMA Volumes in Mathematics and its Applications, Volume 58, pp. 33–47. New York: Springer-Verlag, 1993.



To integrate $du/dt = f(u)$ from $t = t_n$ to $t_{n+1} = t_n + \Delta t$, we first apply the trapezoidal rule (TR) to advance the solution from t_n to $t_{n+\gamma} = t_n + \gamma\Delta t$:

$$u_{n+\gamma} - \gamma\frac{\Delta t}{2} f_{n+\gamma} = u_n + \gamma\frac{\Delta t}{2} f_n, \tag{1}$$

and then use the second-order backward differentiation formula (BDF2)[1] to advance the solution to t_{n+1}:

$$u_{n+1} - \frac{1-\gamma}{2-\gamma}\Delta t\, f_{n+1} = \frac{1}{\gamma(2-\gamma)} u_{n+\gamma} - \frac{(1-\gamma)^2}{\gamma(2-\gamma)} u_n. \tag{2}$$

This composite one-step method is second-order accurate and L-stable.

We linearize f_{n+1} in Eq. (2) (and similarly $f_{n+\gamma}$ in Eq. (1)) iteratively by setting the new iterative solution to

$$u_{n+1}^{(k+1)} = u_{n+1}^{(k)} + \delta u^{(k)}, \quad u_{n+1}^{(0)} = u_{n+\gamma} \tag{3}$$

and approximating

$$f_{n+1}^{(k+1)} = f_{n+1}^{(k)} + \left(\frac{\partial f}{\partial u}\right)_{n+1}^{(k)} \delta u^{(k)} \tag{4}$$

[1]For BDF2, $e_l \approx -\frac{(1-\gamma)^2}{6(2-\gamma)}\Delta t^3 u'''$.

where $k = 0,\ 1,\ \ldots$ labels the Newton iterations. At each TR or BDF2 partial step, we iterate until the Newton method converges.

The Newton equation for the TR partial step is

$$\left[I - \gamma \frac{\Delta t}{2} \left(\frac{\partial f}{\partial u} \right)^{(k)}_{n+\gamma} \right] \delta u^{(k)} = - \left(u^{(k)}_{n+\gamma} - u_n \right) + \gamma \frac{\Delta t}{2} \left(f^{(k)}_{n+\gamma} + f_n \right) \equiv -R_{\rm TR} \tag{5}$$

where $R_{\rm TR}$ is the residual for Eq. (1).

The Newton equation for the BDF2 partial step is

$$\left[I - \frac{1-\gamma}{2-\gamma} \Delta t \left(\frac{\partial f}{\partial u} \right)^{(k)}_{n+1} \right] \delta u^{(k)} =$$

$$- \left(u^{(k)}_{n+1} - \frac{1}{\gamma(2-\gamma)} u_{n+\gamma} + \frac{(1-\gamma)^2}{\gamma(2-\gamma)} u_n \right) + \frac{1-\gamma}{2-\gamma} \Delta t f^{(k)}_{n+1} \equiv -R_{\rm BDF2} \tag{6}$$

where $R_{\rm BDF2}$ is the residual for Eq. (2).

The timestep size Δt is adjusted dynamically within a window $[\Delta t_{\rm min}, \Delta t_{\rm max}]$ by monitoring a divided-difference estimate of the local error e_l:

$$e_l = k_\gamma \Delta t^3 u''' \tag{7}$$

$$\approx 2 k_\gamma \Delta t \left(\frac{1}{\gamma} f_n - \frac{1}{\gamma(1-\gamma)} f_{n+\gamma} + \frac{1}{1-\gamma} f_{n+1} \right), \tag{8}$$

where

$$k_\gamma = \frac{-3\gamma^2 + 4\gamma - 2}{12(2-\gamma)}. \tag{9}$$

The three values of f employed in Eq. (8) have already been calculated in the most recent TRBDF2 timestep. The $||e_l||$ is minimized for $\gamma = 2 - \sqrt{2}$.

A-stability and L-stability

A time integration method for $du/dt = au$ ($\mathrm{Re}\{a\} < 0$) is **A-stable** if

$$\frac{||u_{n+1}||}{||u_n||} = ||G|| \leq 1 \tag{10}$$

for all $\Delta t > 0$. A time integration method for $du/dt = au$ ($\mathrm{Re}\{a\} < 0$) is **L-stable** if it is A-stable and

$$\lim_{\Delta t \to \infty} \frac{||u_{n+1}||}{||u_n||} = \lim_{\Delta t \to \infty} ||G|| = 0. \tag{11}$$

TR is A-stable, but not L-stable. Backward Euler (first- and second-order) and TRBDF2 are L-stable.

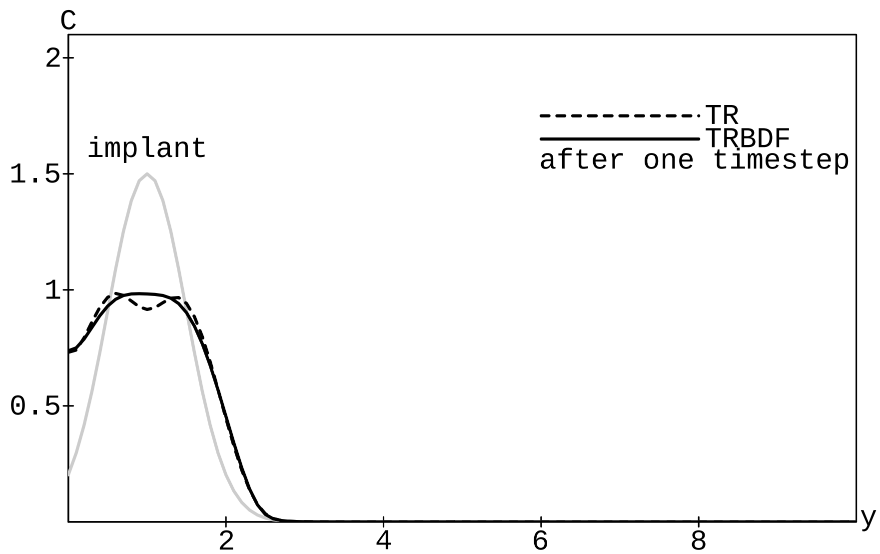


Figure 1: Simulation of nonlinear diffusion in semiconductor processing with a large Δt.

The growth factor G for TRBDF2 for $du/dt = -\alpha u$, $\alpha > 0$ is given by ($\Delta \equiv \gamma\alpha\Delta t > 0$):

$$G(\Delta t, \gamma) = \frac{\frac{1-\frac{\gamma\alpha\Delta t}{2}}{1+\frac{\gamma\alpha\Delta t}{2}} - (1-\gamma)^2}{\gamma(2-\gamma) + \gamma(1-\gamma)\alpha\Delta t} = \frac{\frac{2-\Delta}{2+\Delta} - (1-\gamma)^2}{\gamma(2-\gamma) + (1-\gamma)\Delta}.$$

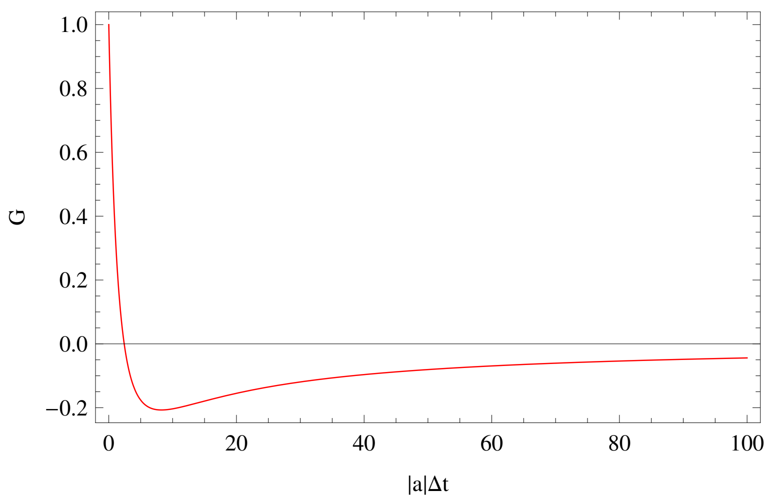


Figure 2: G_{TRBDF2} as a function of $|a|\Delta t$ for $\gamma = 2 - \sqrt{2}$.