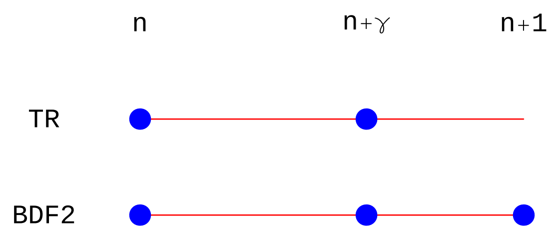
TRBDF2

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 $t_{n+1} = t_n + \Delta t_n$, we first apply the trapezoidal rule (TR) to advance the solution from t_n to $t_{n+\gamma} = t_n + \gamma \Delta t_n$:

$$u^{n+\gamma} \; - \; \gamma \frac{\Delta t_n}{2} f^{n+\gamma} = u^n \; + \; \gamma \frac{\Delta t_n}{2} f^n \; , \tag{1}$$

and then use the second-order backward differentiation formula (BDF2) to advance the solution from $t_{n+\gamma}$ to t_{n+1}:

$$u^{n+1} \; - \; \frac{1-\gamma}{2-\gamma} \Delta t_n f^{n+1} = \frac{1}{\gamma(2-\gamma)} u^{n+\gamma} \; - \; \frac{(1-\gamma)^2}{\gamma(2-\gamma)} u^n \; . \tag{2}$$

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)) by approximating

$$f^{n+1}_{(k+1)} = f^{n+1}_{(k)} \; + \; \left(\frac{\partial f}{\partial u} \right)^{n+1}_{(k)} \delta u^{n+1}_{(k)} \tag{3}$$

where $k = 0, \; 1, \; \ldots$ labels the Newton iterations. The new solution is obtained by setting

$$u^{n+1}_{(k+1)} = u^{n+1}_{(k)} \; + \; \lambda \delta u^{n+1}_{(k)} \; , \quad u^{n+1}_{(0)} = u^{n+\gamma} \tag{4}$$

where λ is a damping factor between 0 and 1, chosen to insure that the norm of the residual for Eq. (1) or (2) decreases monotonically. At each TR or BDF2 partial step, we iterate until the Newton method converges.

The Newton equation for the TR partial step is

$$\left[1 \;-\; \gamma\frac{\Delta t_n}{2}\left(\frac{\partial f}{\partial u}\right)^{n+\gamma}_{(k)}\right]\delta u^{n+\gamma}_{(k)} = -\,(u^{n+\gamma}_{(k)} \;-\; u^n) \;+\; \gamma\frac{\Delta t_n}{2}(f^{n+\gamma}_{(k)} \;+\; f^n) \;\equiv\; -R_{\rm TR} \tag{5}$$

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

The Newton equation for the BDF2 partial step is

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

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

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 truncation error LTE:

$$\text{LTE}^{n+1} \;=\; k\Delta t_n^3 u^{(3)} \tag{7}$$

$$\approx\; 2k\Delta t_n\left(\frac{1}{\gamma}f^n - \frac{1}{\gamma(1-\gamma)}f^{n+\gamma} + \frac{1}{1-\gamma}f^{n+1}\right), \tag{8}$$

where

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

The three values of f employed in Eq. (8) have already been calculated in the most recent TRBDF2 timestep.

The $|LTE|$ is minimized for $\gamma = 2 - \sqrt{2}$.

A-stability and L-stability

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

$$||u^{n+1}|| \leq ||u^n||. \tag{10}$$

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

$$\lim_{\Delta t\to\infty}\frac{||u^{n+1}||}{||u^n||} = 0. \tag{11}$$

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

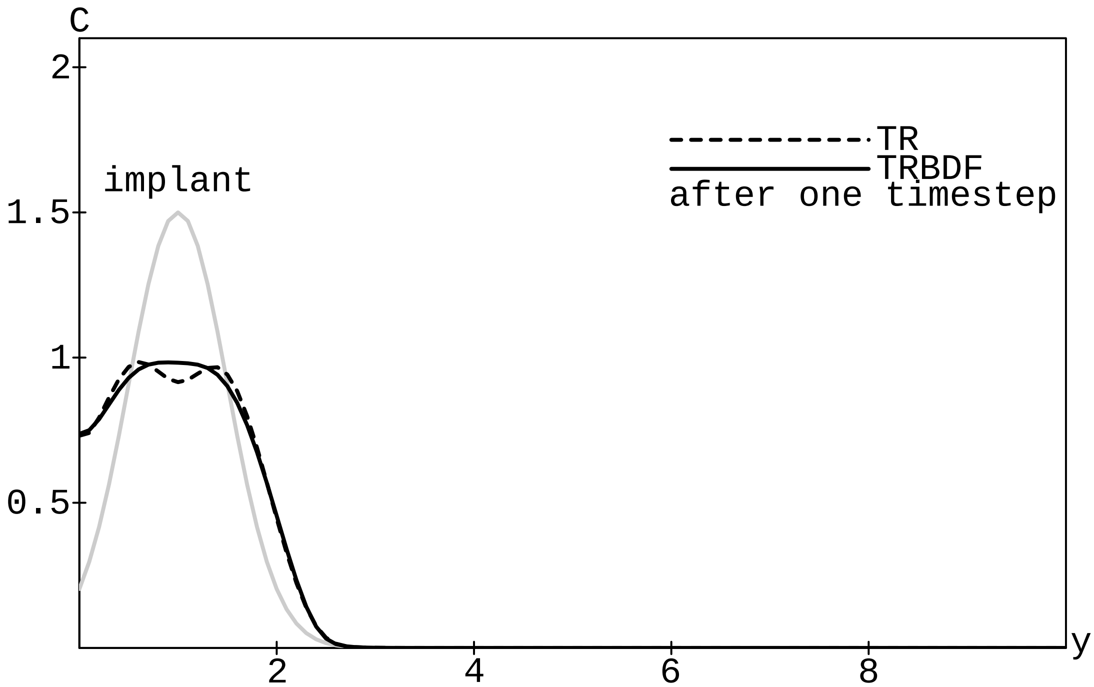


Figure 1: Simulation of nonlinear diffusion in semiconductor processing with a large Δt.