Executing models in less time—some solver insight

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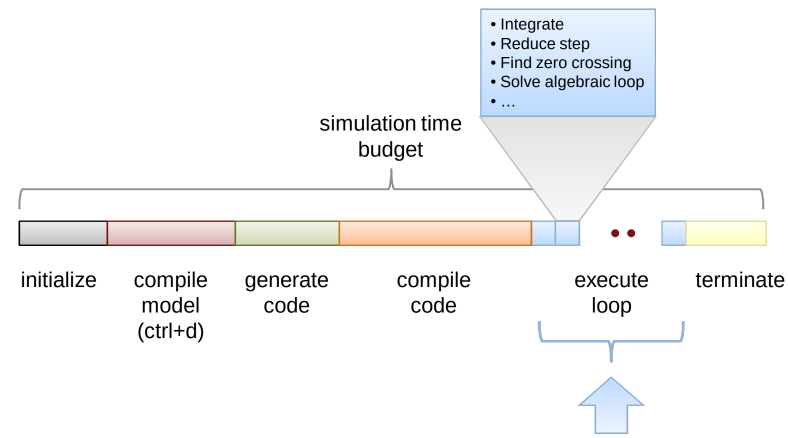
What all may affect simulation performance?

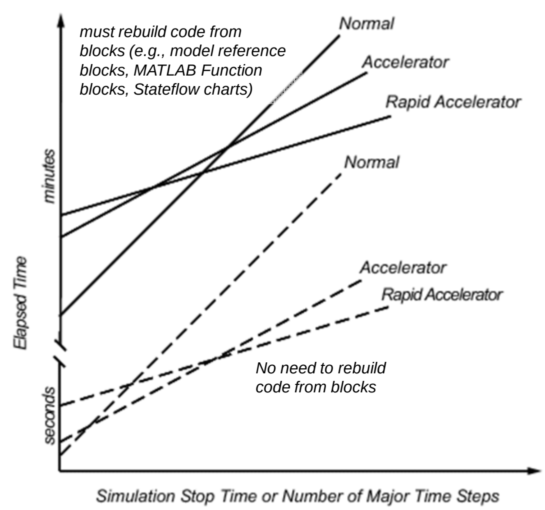
- Model
  - Initialization (images, ML script, set_params, …)
  - Execution
  - Code generation
- **Solver**
- Processing (Engine, Code Generator, Compiler)
  - Optimization
  - Diagnostics
- Interaction
  - Debugging
  - Logging
  - Viewing
- Simulation mode
- Platform
- Use scenarios
  - Simstate

http://www.mathworks.com/company/events/webinars/webinarconf.html?id=54186&language=en

The make up of a simulation



Comparing performance of different simulation modes

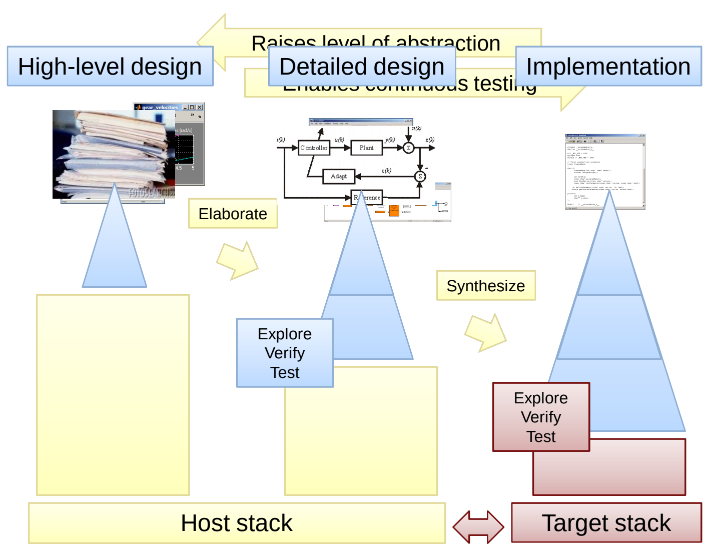


Help Search: comparing performance

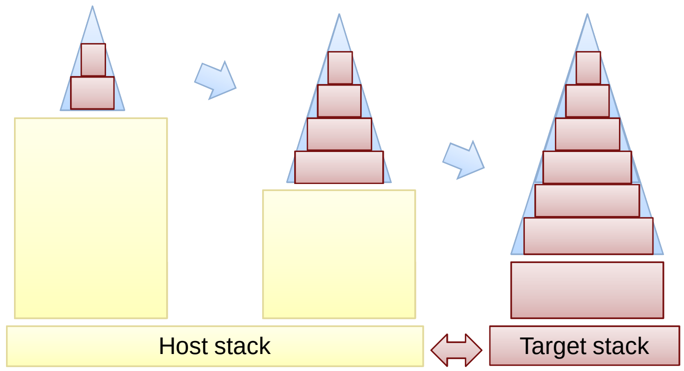
Agenda

- Constructing models with increasing fidelity
- Execution of models explained
  - Fixed step solver methods
  - Variable step solver methods
  - Zero crossings
- Conclusions

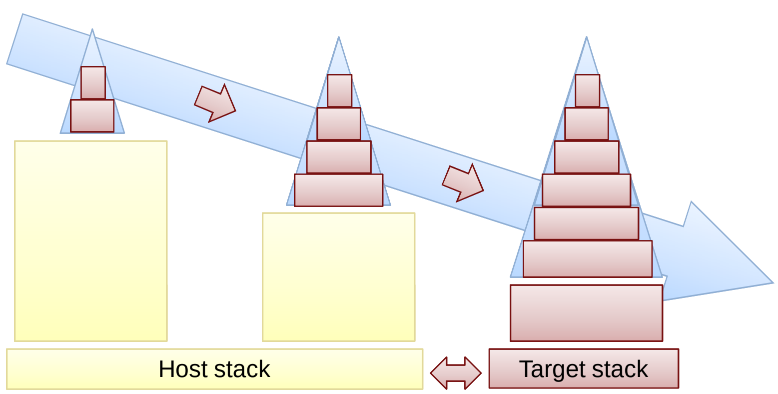
Model-Based Design



Create executable models in all phases



Make the computational approximation the primary design deliverable—the real thing!



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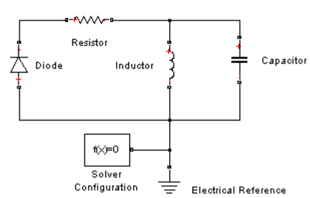
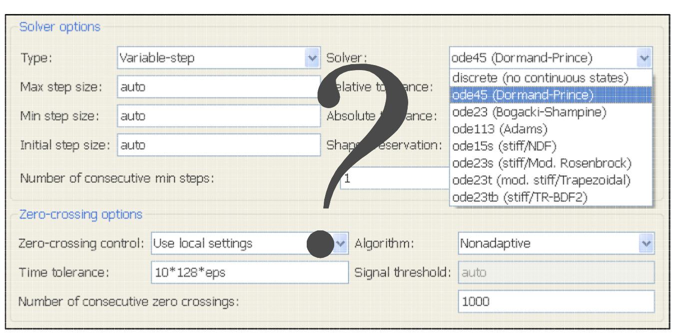
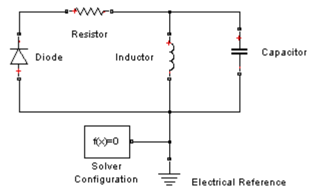
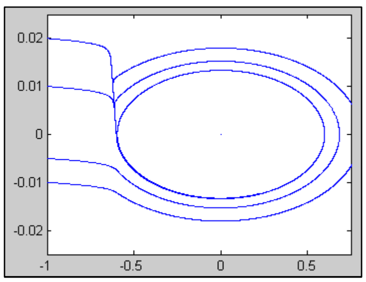
A Simscape model—what solver to choose?

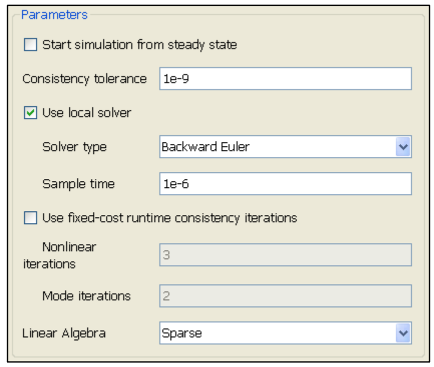




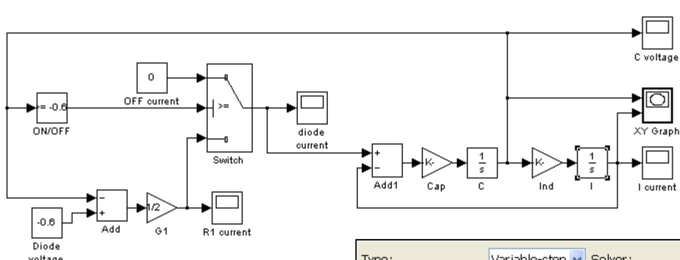
Using a Simscape solver to generate reference behavior

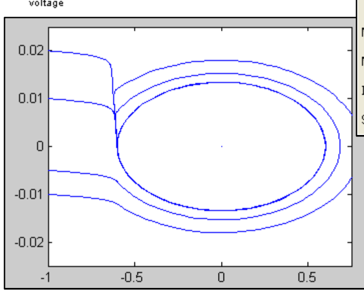


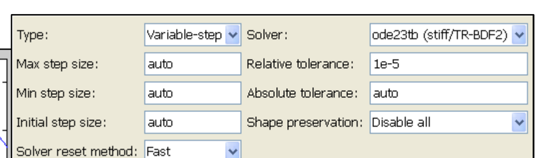




The corresponding Simulink model with an ideal diode







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ode1: forward Euler numerical integration

Step h in time

$$h_k = t_{k+1} - t_k$$

Along instantaneous vector component

$$\dot{x} = f(x,t)$$

Gives the estimate

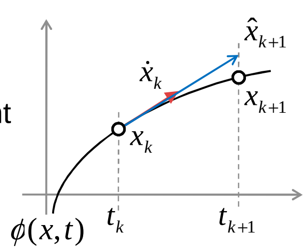
$$\hat{x}_e(t_{k+1}) = x(t_k) + \dot{x}(t_k)h_k$$

Comparison with Taylor series expansion

$$x(t_{k+1}) = x(t_k) + \frac{\dot{x}(t_k)}{1!}h_k + \frac{\ddot{x}(t_k)}{2!}h_k^2 + O(h_k^3)$$

Gives error of the estimate

$$\varepsilon(t_{k+1}) = O(h_k^2)$$



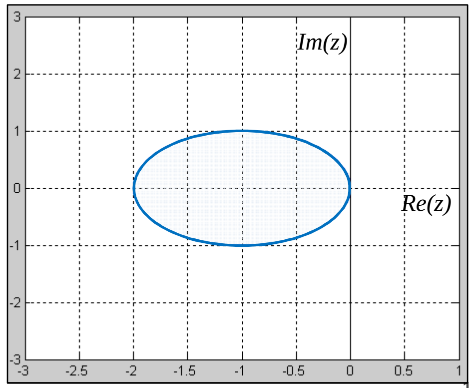
ode1: stability analysis

$$\dot{x} = kx; \quad x(0) = 1 \qquad\qquad x(t) = e^{kt}$$

$$\hat{x}_e(t_{k+1}) = x(t_k) + \dot{x}(t_k) h_k$$

$$\hat{x}_e(t_{k+1}) = \hat{x}_e(t_k) + kh\hat{x}_e(t_k) \Rightarrow \hat{x}_e(t_{k+n}) = (1+kh)^n \hat{x}_e(t_k)$$

$$k \in C, z = kh \Rightarrow \{z \in C \,|\, |1+z| < 1\}$$



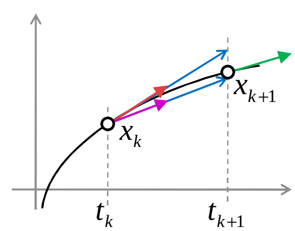
In MATLAB:

```
>> clear i
>> [X,Y]= meshgrid(-3:0.01:1,-3:0.01:3);
>> Mu = X + i*Y;
>> R = 1 + Mu;
>> Rhat = abs(R);
>> contour(X,Y,Rhat,[1, 1],'b')
>> grid
>> hold
>> plot([0 0],[-3 3],'k')
```


Trapezoidal numerical integration

Average beginning and end point

$$\boxed{\hat{x}_t(t_{k+1})} = x(t_k) + \boxed{\frac{\dot{x}(t_{k+1}) + \dot{x}(t_k)}{2}} h_k$$



Finite difference …

$$\ddot{x}(t_k) = \frac{\dot{x}(t_{k+1}) - \dot{x}(t_k)}{h_k} + O(h_k)$$

… to approximate Taylor series expansion

$$x(t_{k+1}) = \underbrace{\boxed{x(t_k) + \frac{\dot{x}(t_k)}{1!} h_k + \frac{\ddot{x}(t_k)}{2!} h_k^2}}_{\hat{x}_t(t_{k+1})} + \underbrace{\boxed{O(h_k^3)}}_{\varepsilon(t_{k+1})}$$

$$x(t_{k+1}) = x(t_k) + \dot{x}(t_k) h_k + \frac{\dot{x}(t_{k+1}) - \dot{x}(t_k)}{2} h_k + O(h_k^3)$$

ode2: Heun method

- But, we do not have the value at t_{k+1} because that is what we are trying to compute
- So, combine trapezoidal with Euler approximation

$$\hat{x}_t(t_{k+1}) = x(t_k) + \frac{\dot{x}(t_{k+1}) + \dot{x}(t_k)}{2} h_k$$

$$\dot{x}(t_k) = f\left(x(t_k), t_k\right)$$

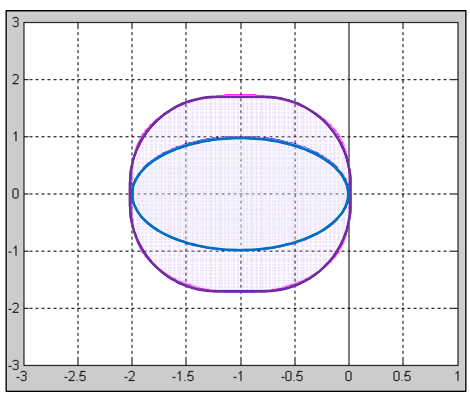
$$\dot{x}(t_{k+1}) = f\left(\boxed{x(t_k) + h\dot{x}(t_k)}, t_{k+1}\right)$$

ode2: (Heun) stability

$$k \in C, z = kh \Rightarrow \left\{ z \in C \,|\, \left|1 + z + \frac{1}{2} z^2\right| < 1 \right\}$$

In MATLAB:

```
>> clear i
>> [X,Y]= meshgrid(-3:0.01:1,-3:0.01:3);
>> Mu = X + i*Y;
>> R = 1 + Mu;
>> Rhat = abs(R);
>> contour(X,Y,Rhat,[1, 1],'b')
>> grid
>> hold
>> plot([0 0],[-3 3],'k')
>> R = 1 + Mu + .5*Mu.^2;
>> Rhat = abs(R);
>> contour(X,Y,Rhat,[1, 1],'m')
```



Stability area of Runge-Kutta methods increases with order

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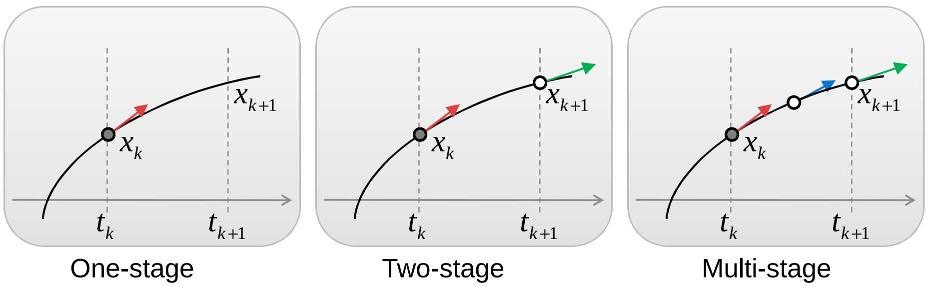
In general, varying order of numerical solvers

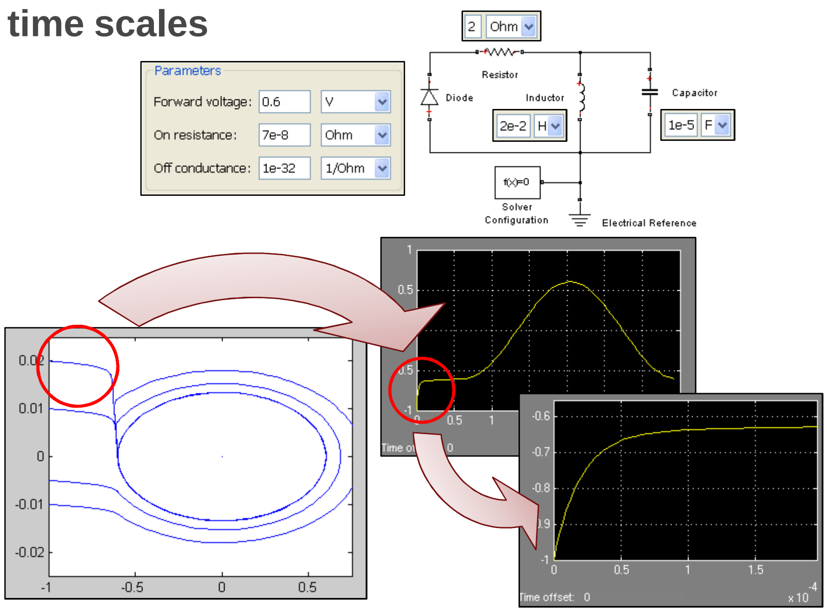


For example: ode1, ode2, ode3, ode4, ode5, ode8

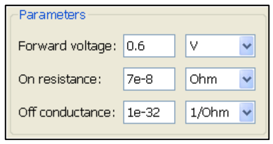
More accurate and stable as order increases

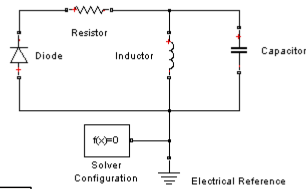
MathWorks

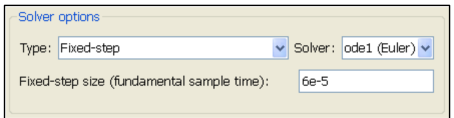
Stiff systems mix behavior at widely differing time scales

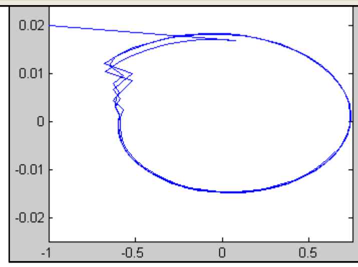


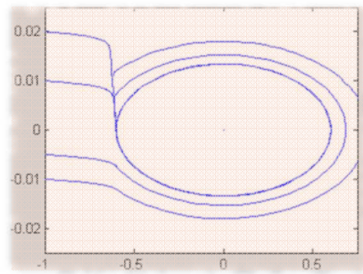
Fixed step and solver order must be chosen carefully—ode1, 6e-5











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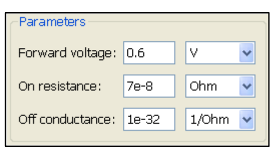
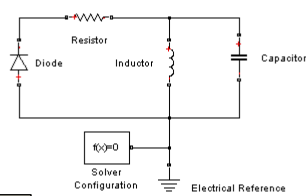
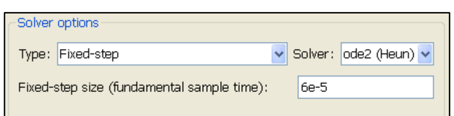
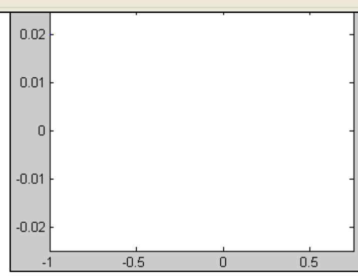
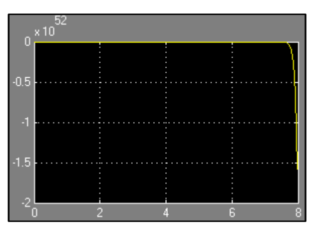
Fixed step and solver order must be chosen carefully—ode2, 6e-5











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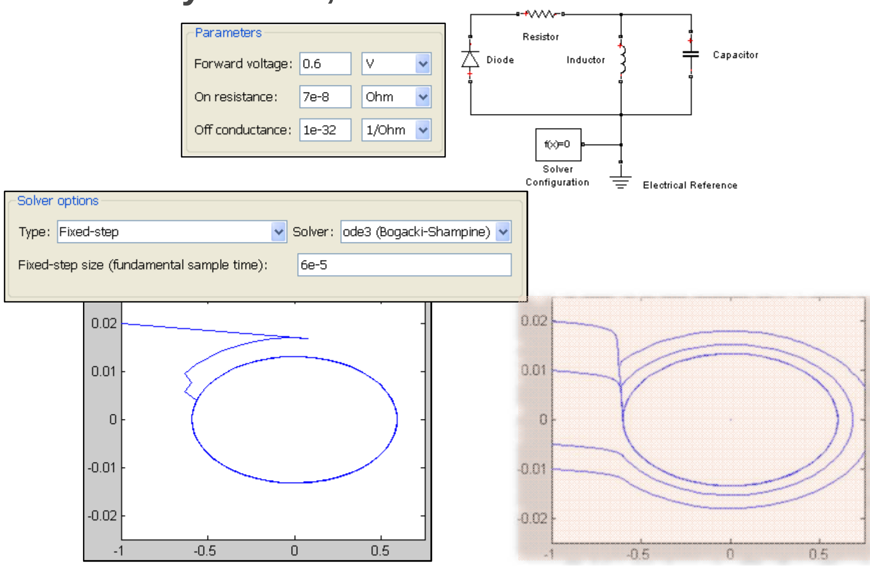
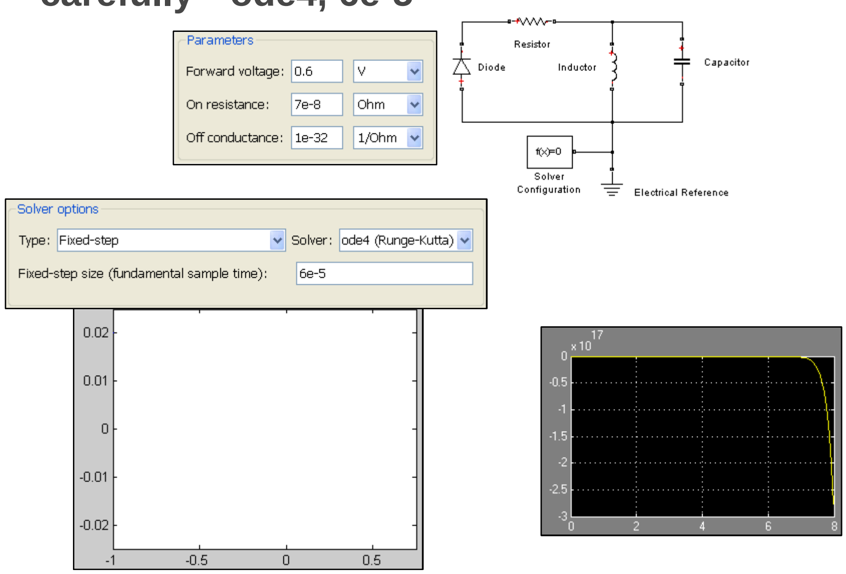
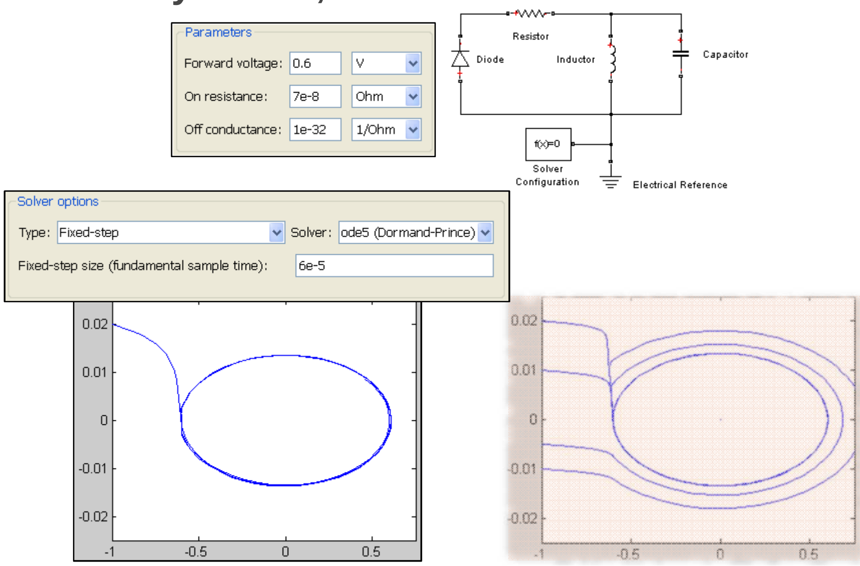
Fixed step and solver order must be chosen carefully—ode3, 6e-5



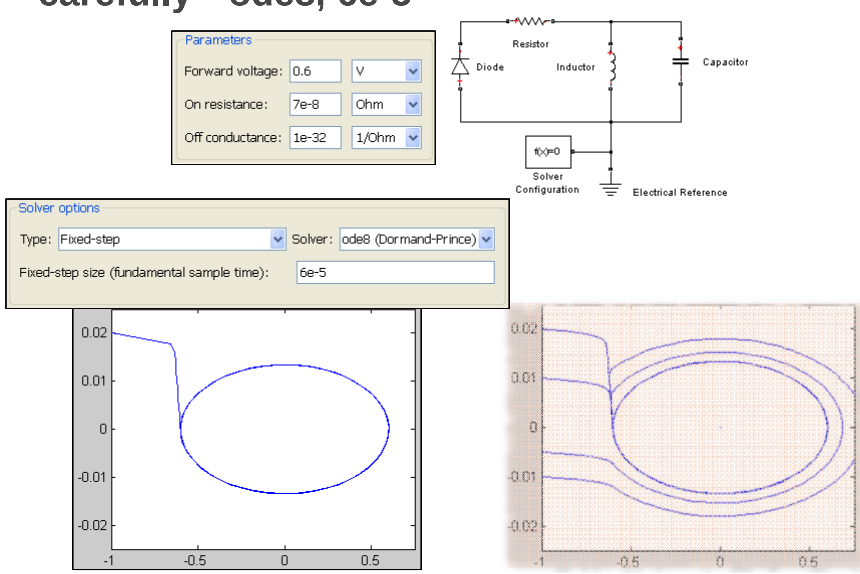
Fixed step and solver order must be chosen carefully—ode4, 6e-5



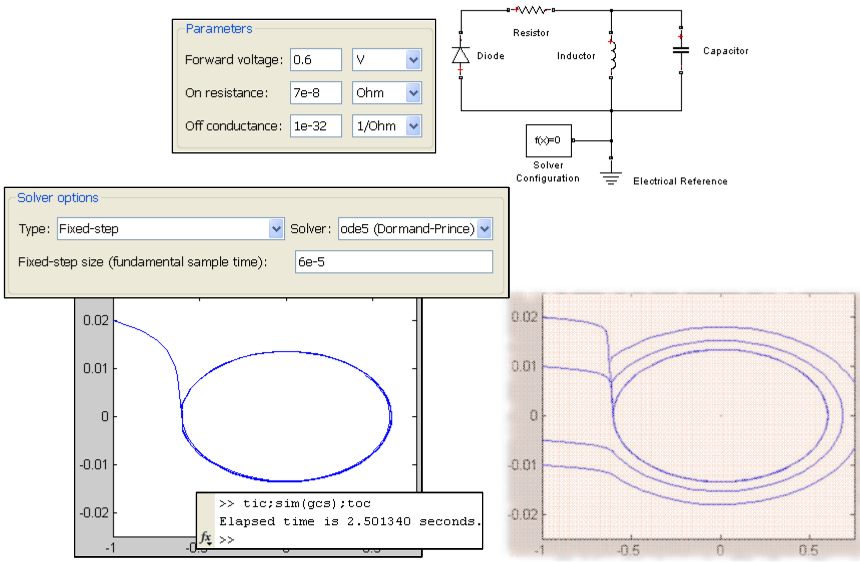
Fixed step and solver order must be chosen carefully—ode5, 6e-5



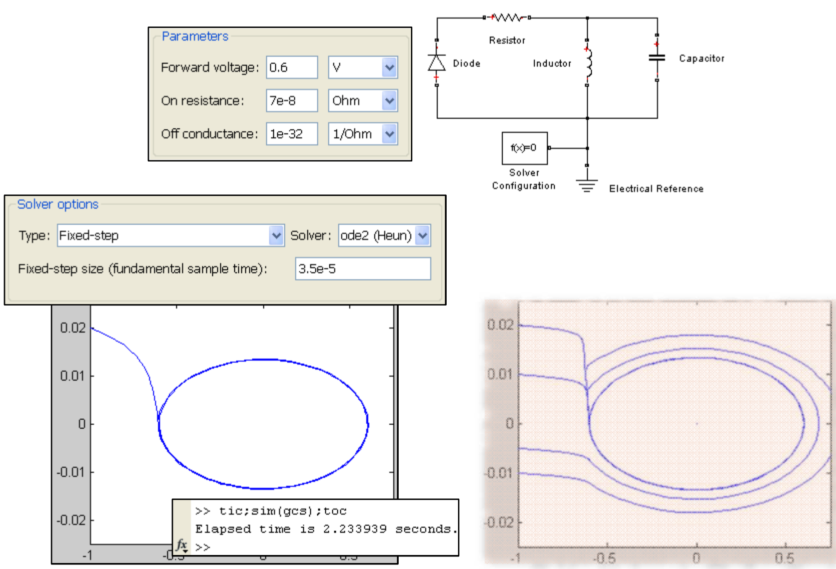
Fixed step and solver order must be chosen carefully—ode8, 6e-5



Step size and order determine simulation time



Step size and order determine simulation time



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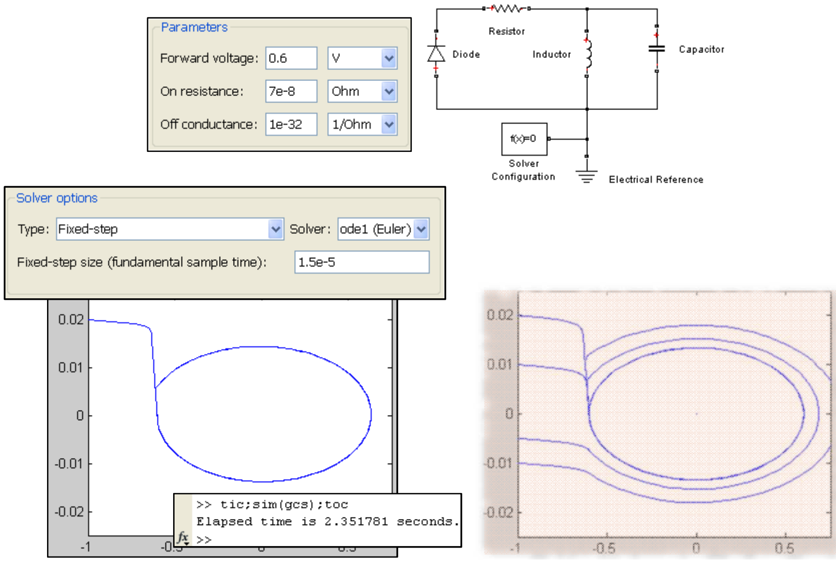
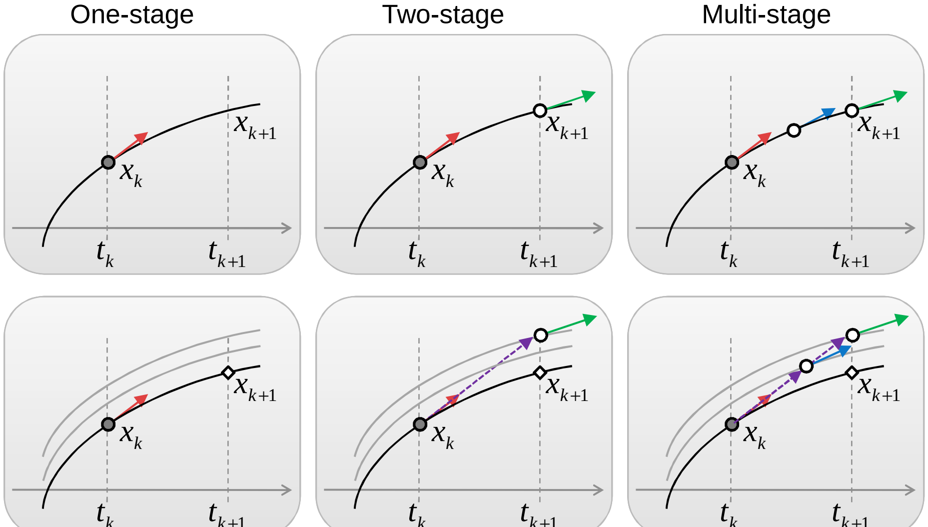
Step size and order determine simulation time



MathWorks

But these solvers really used an explicit formulation

One-stage Two-stage Multi-stage



How about a truly implicit approach?

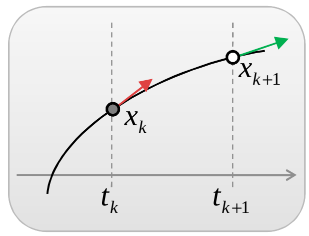
- Trapezoidal integration
  - Requires future points!
  - Impossible?
- Can do, but requires inverting the system

$$\hat{x}_t(t_{k+1}) = x(t_k) + \frac{\dot{x}(t_{k+1}) + \dot{x}(t_k)}{2} h_k$$

$$\hat{x}_t(t_{k+1}) = \hat{x}_t(t_k) + \frac{A\hat{x}_t(t_{k+1}) + A\hat{x}_t(t_k)}{2} h_k$$

$$(2I - Ah)\hat{x}_t(t_{k+1}) = (2I + Ah)\hat{x}_t(t_k)$$

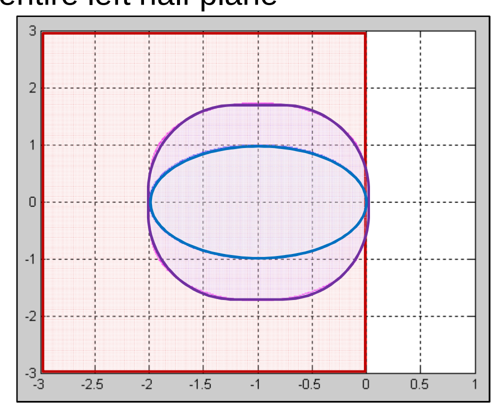
$$\hat{x}_t(t_{k+1}) = (2I - Ah)^{-1}(2I + Ah)\hat{x}_t(t_k)$$



Plusses and deltas?

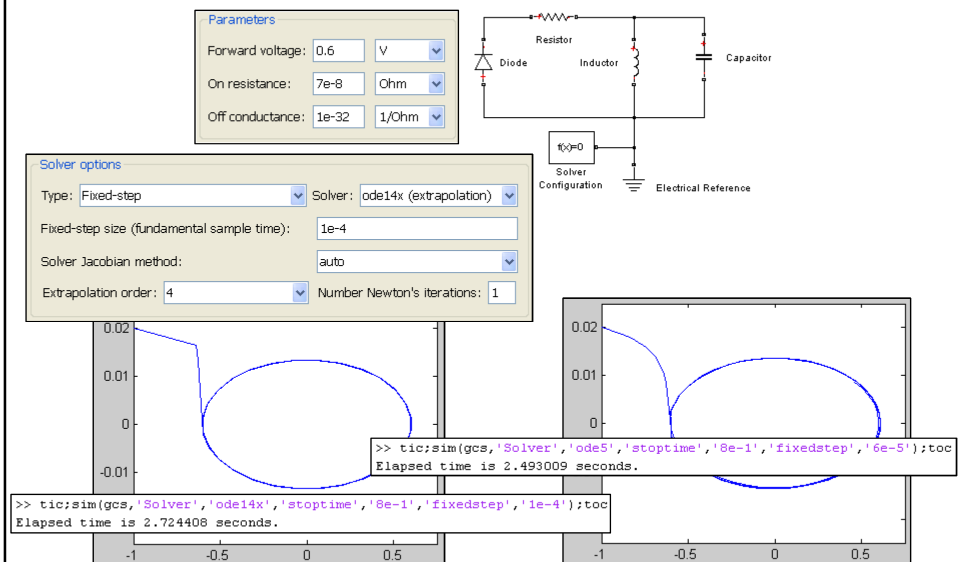
- Trapezoidal is stable in entire left half plane

In MATLAB:
```
>> clear i
>> [X,Y]= meshgrid(-3:0.01:1,-3:0.01:3);
>> Mu = X + i*Y;
>> R = 1 + Mu;
>> Rhat = abs(R);
>> contour(X,Y,Rhat,[1, 1],'b')
>> grid
>> hold
>> plot([0 0],[-3 3],'k')
>> R = 1 + Mu + .5*Mu.^2;
>> Rhat = abs(R);
>> contour(X,Y,Rhat,[1, 1],'m')
>> R = (2 + Mu)./(2-Mu);
>> Rhat = abs(R);
>> contour(X,Y,Rhat,[1, 1],'r')
```

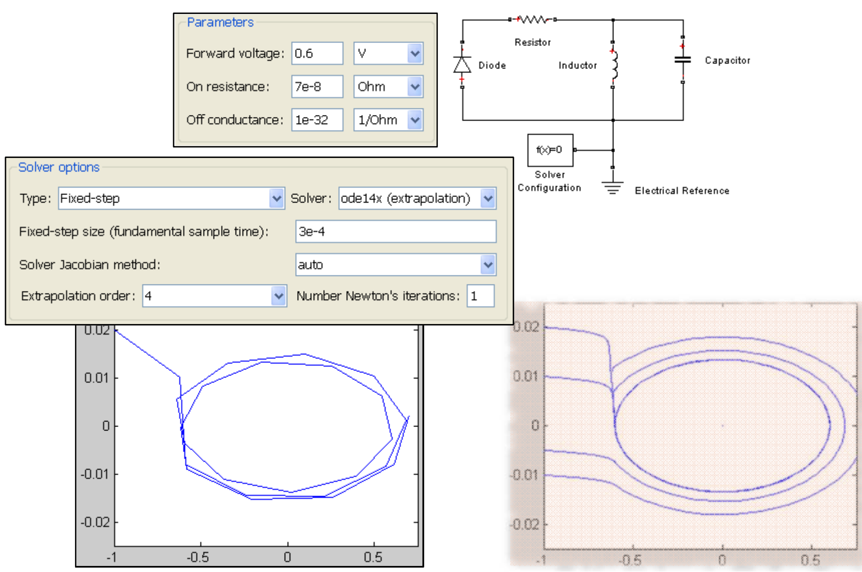


- But, expensive!
  - Linearization
  - Inversion

Advantage: a large step size is possible



Still stable with very large step size



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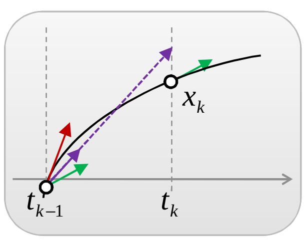
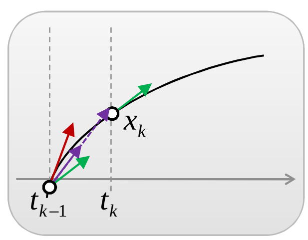
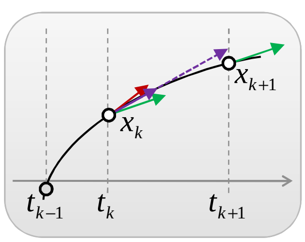
A fixed step size has to be stable for the fastest behavior anywhere in a simulation

From k-1 to k
Fast behavior, so a small step is necessary





From k to k+1
Slow behavior, so a large step is possible



Is the ‘fast’ behavior holding us hostage?

Step size control

- Compute Euler approximation

$$\hat{x}_e(t_{k+1}) = x(t_k) + f\big(x(t_k)\big)h_k$$

- Compute Heun approximation

$$\hat{x}_t(t_{k+1}) = x(t_k) + \frac{f\big(\hat{x}_e(t_{k+1})\big) + f\big(x(t_k)\big)}{2} h_k$$

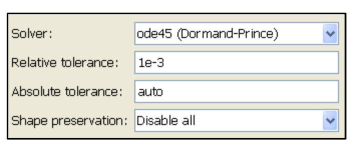
- Compare the results for the error estimate, ε

$$x_e(t_{k+1}) - x_t(t_{k+1}) \approx \frac{\ddot{x}(t_k)}{2!} h_k^2 = \varepsilon_e(t_{k+1})$$

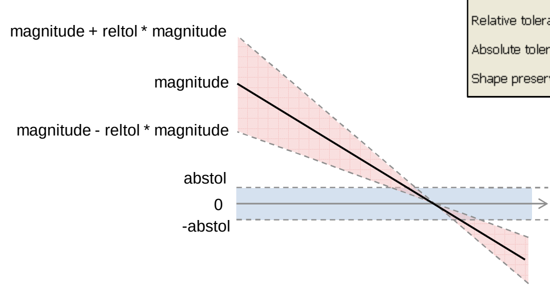
- Reduce step size from h_{max} till $\varepsilon < tol$
  - For example, bisection

Tolerance consists of two components

- Relative tolerance depends on signal magnitude
- Absolute tolerance is constant

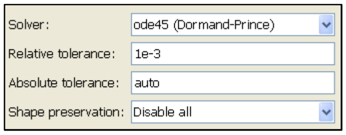


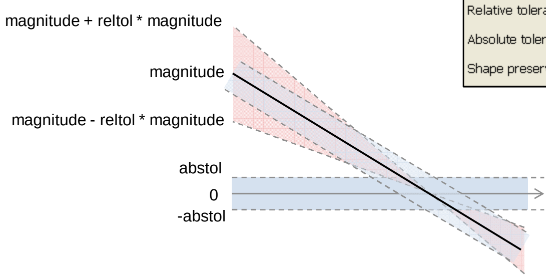
Solver:	ode45 (Dormand-Prince)
Relative tolerance:	1e-3
Absolute tolerance:	auto
Shape preservation:	Disable all



Approximations determined by absolute and relative tolerance

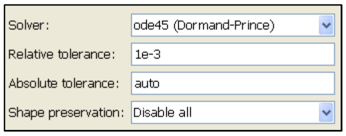
- Absolute tolerance prevents infinitely accurate solution around 0

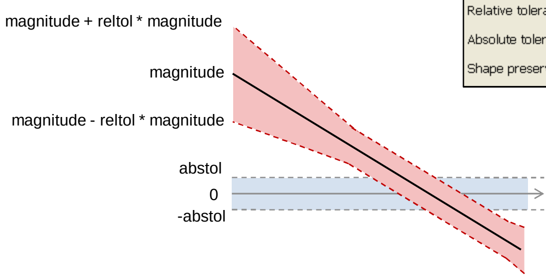




Approximations determined by absolute and relative tolerance

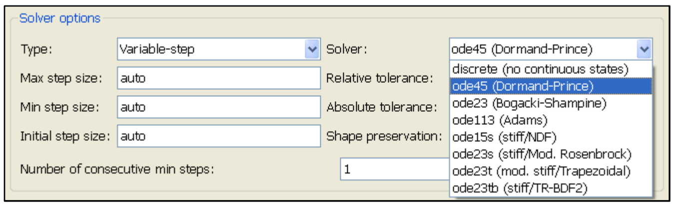
- Combined relative and absolute tolerance drive solver step size selection





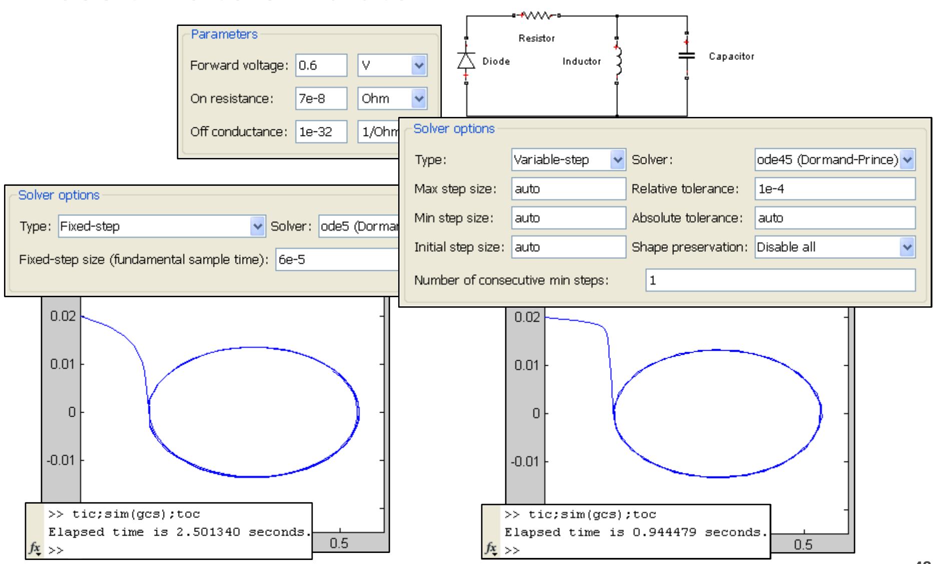
Variable step solvers

- ode45
  - Compares RK methods of order 4 and 5
- ode23
  - Compares RK methods of order 2 and 3
- ode23tb
  - Trapezoidal (implicit) integration with BDF error estimate

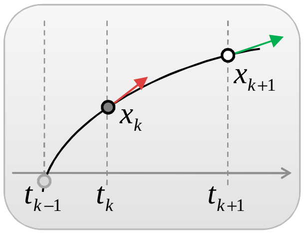


But now we better be careful with our computational complexity?

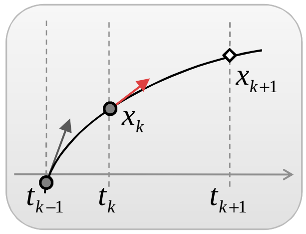
A variable-step solver may actually take much less time to simulate



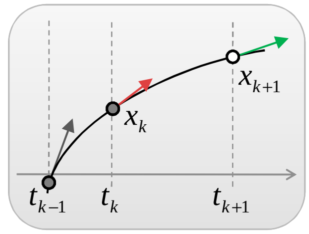
And we can do even better: multi-step solvers reuse effort



Implicit multi-stage
(e.g., ode23tb, ode23t)

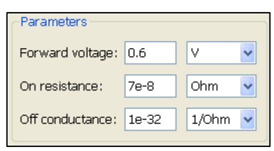


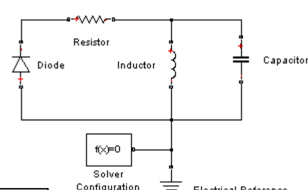
Explicit multi-step
(e.g., ode113)



Implicit multi-step
(e.g., ode15s)

So, yet more efficient integration





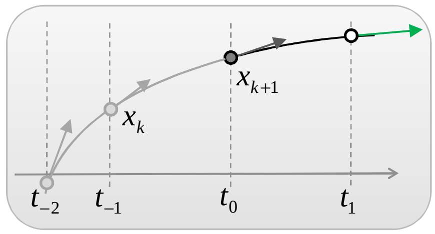

```
>> tic;sim(gcs,'reltol','1e-4','Solver','ode45','stoptime','0.8');toc
Elapsed time is 1.025632 seconds.
>> tic;sim(gcs,'reltol','1e-4','Solver','ode45','stoptime','0.8');toc
Elapsed time is 0.991488 seconds.
>> tic;sim(gcs,'reltol','1e-4','Solver','ode45','stoptime','0.8');toc
Elapsed time is 1.169297 seconds.
>> tic;sim(gcs,'reltol','1e-4','Solver','ode45','stoptime','0.8');toc
Elapsed time is 1.082161 seconds.
>> tic;sim(gcs,'reltol','1e-4','Solver','ode45','stoptime','0.8');toc
Elapsed time is 1.008882 seconds.
>> tic;sim(gcs,'reltol','1e-4','Solver','ode113','stoptime','0.8');toc
Elapsed time is 0.895317 seconds.
>> tic;sim(gcs,'reltol','1e-4','Solver','ode113','stoptime','0.8');toc
Elapsed time is 0.921423 seconds.
>> tic;sim(gcs,'reltol','1e-4','Solver','ode113','stoptime','0.8');toc
Elapsed time is 0.848121 seconds.
>> tic;sim(gcs,'reltol','1e-4','Solver','ode113','stoptime','0.8');toc
Elapsed time is 0.902069 seconds.
>> tic;sim(gcs,'reltol','1e-4','Solver','ode113','stoptime','0.8');toc
Elapsed time is 0.866556 seconds.
>>
```

ode45: 1.055492

ode113: 0.8866972

multi-stage is ~19% slower than multi-step

But the reuse may turn against us

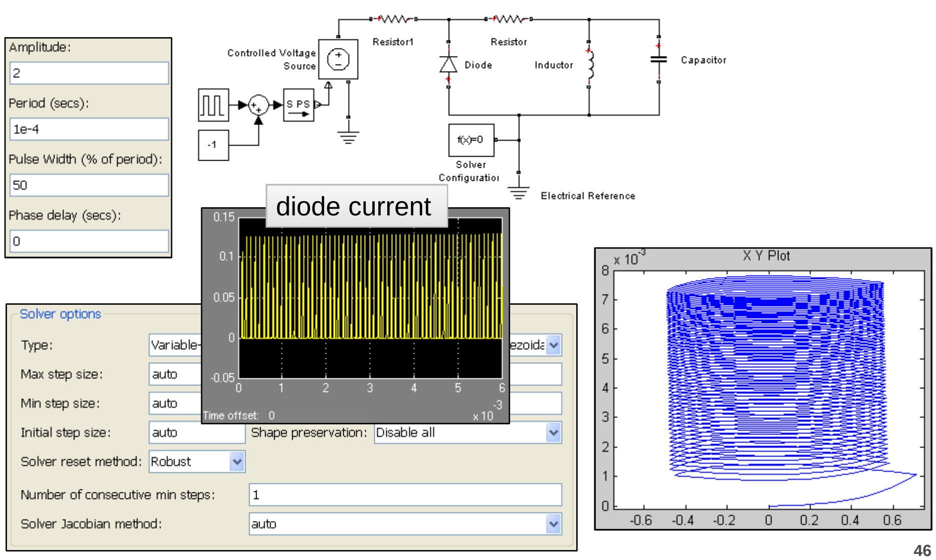


We do not have initial values at t_{-2} and t_{-1}
How do we build this history?
- Single-step integration algorithm
- Either implicit or explicit with very small step size, ε

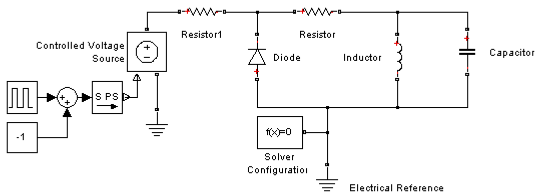
How about t_1 in case of implicit methods?
- Linearize system and invert system matrix

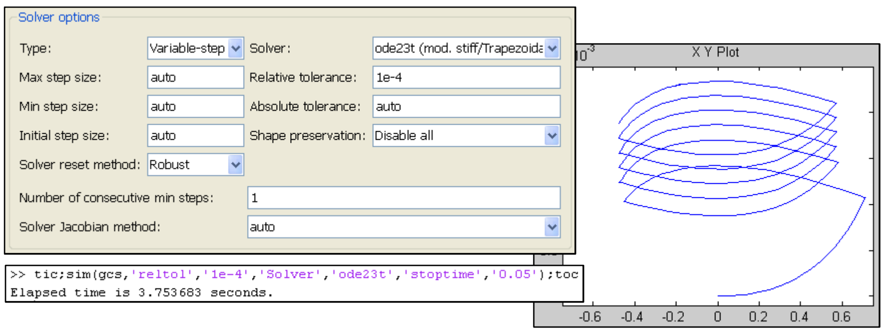
But now when we reach a discontinuity …
… smoothness is violated … solver reset!

Many discontinuities require many solver resets

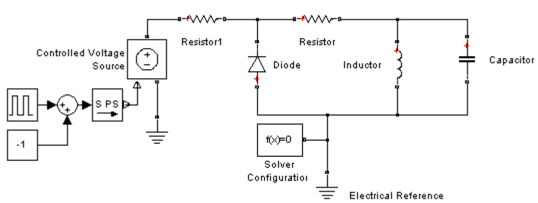


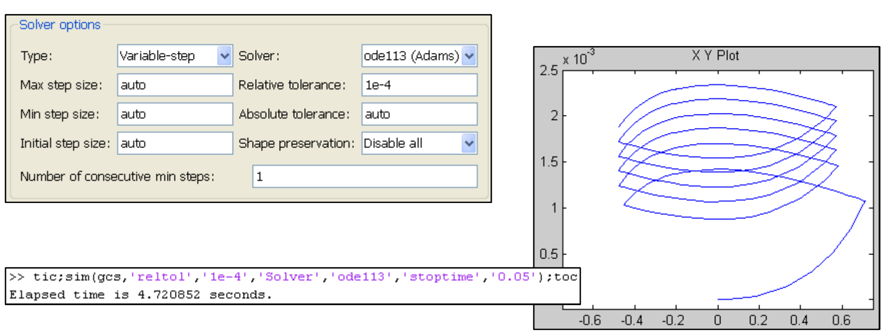
A single-step solver …





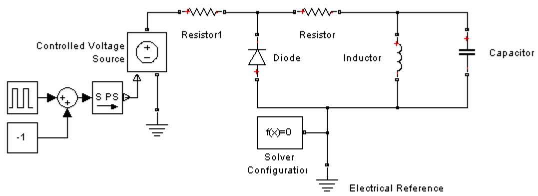
…versus a multi-step solver …

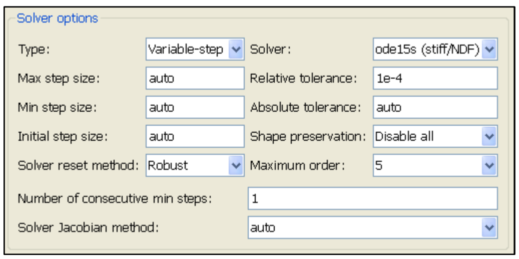




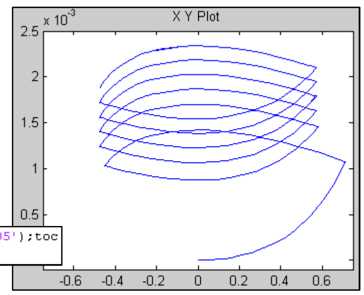
MathWorks

… and another multi-step solver …



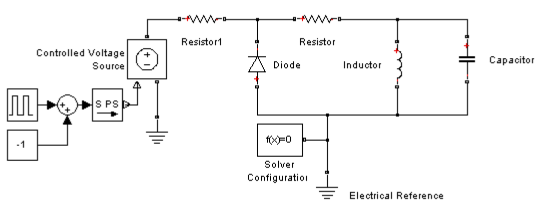


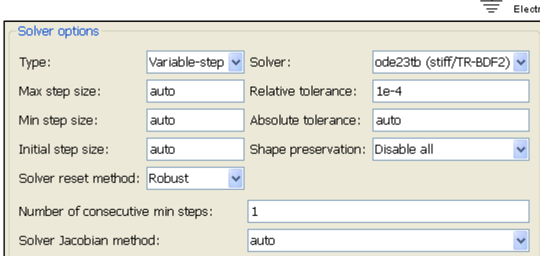

```
>> tic;sim(gcs,'reltol','1e-4','Solver','ode15s','stoptime','0.05');toc
Elapsed time is 4.505691 seconds.
```



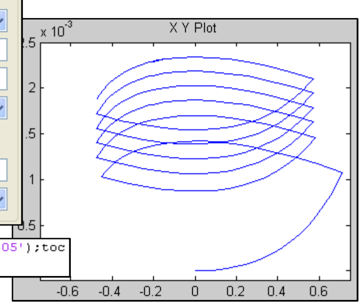
MathWorks

But there is more to it than just the single step nature

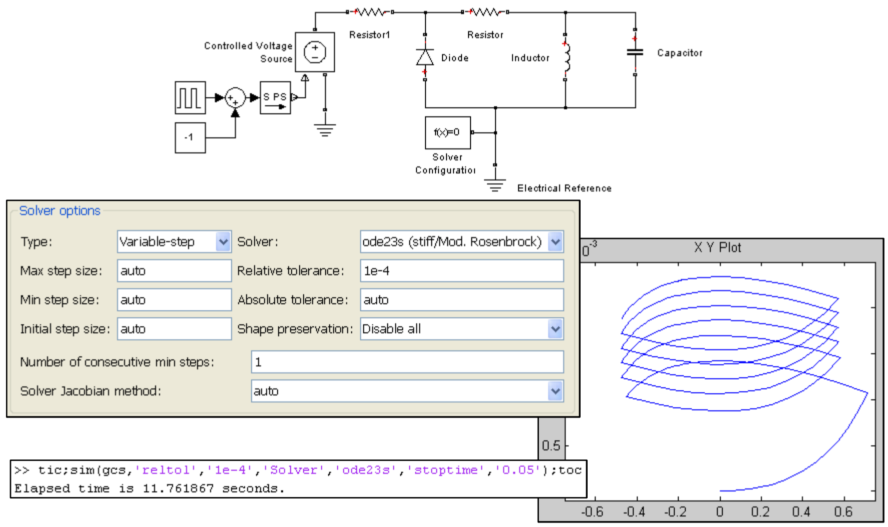




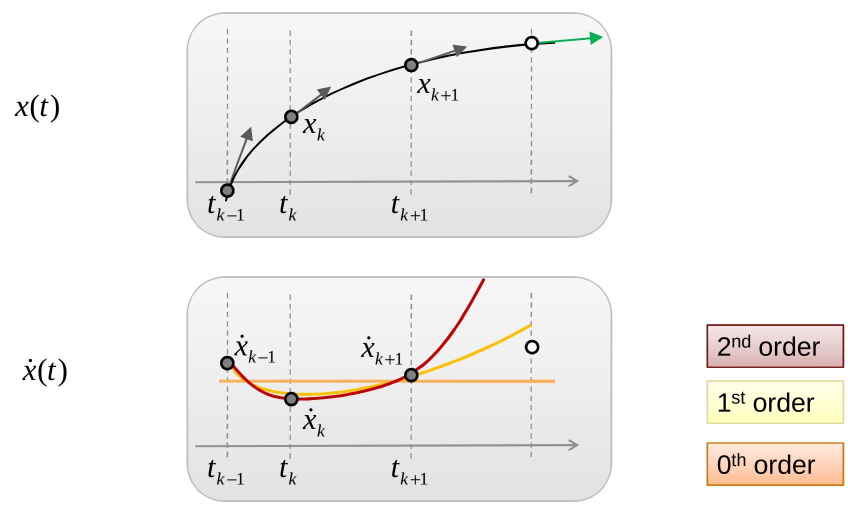

```
>> tic;sim(gcs,'reltol','1e-4','Solver','ode23tb','stoptime','0.05');toc
Elapsed time is 5.529495 seconds.
```



Or even …



Note: extrapolation becomes unreliable for high order



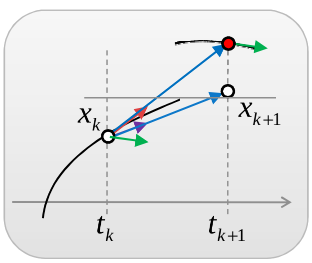
Stability area of multistep methods (explicit: ode113, implicit: ode15s) decreases with order!

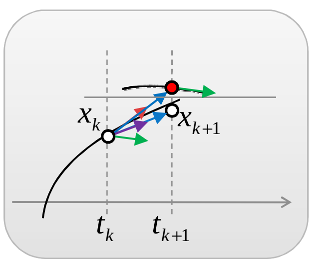
Agenda

- Constructing models with increasing fidelity
- Execution of models explained
  - Fixed step solver methods
  - Variable step solver methods
  - Zero crossings
- Conclusions

Discontinuities

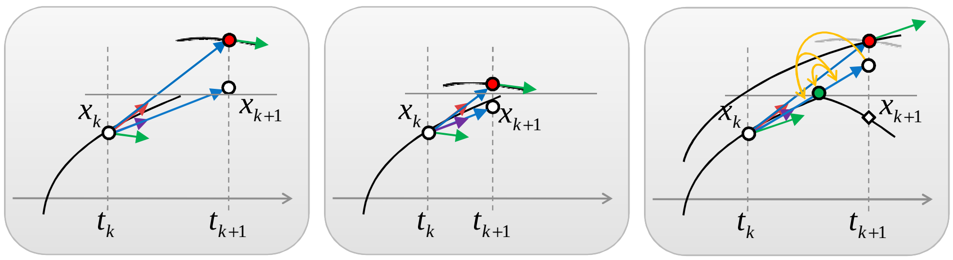
- Variable-step solvers ‘zoom in’ on zero crossings
  - Is solver step size reduction an efficient mechanism?

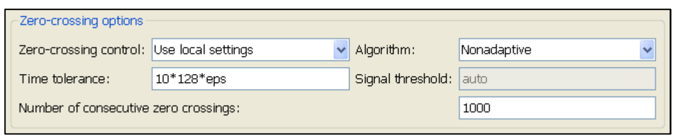




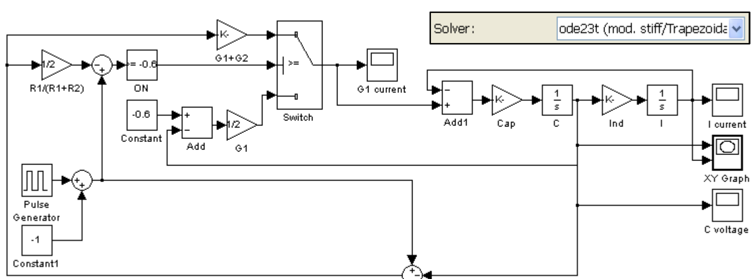
Discontinuities

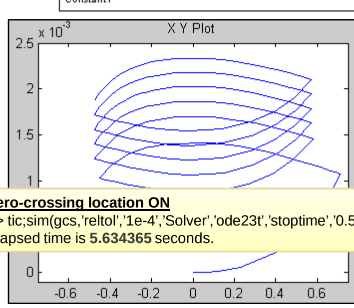
- How about we use a dedicated root-finding algorithm?
  - Bisection, Newton-Raphson
- Disregard the discontinuity, then search



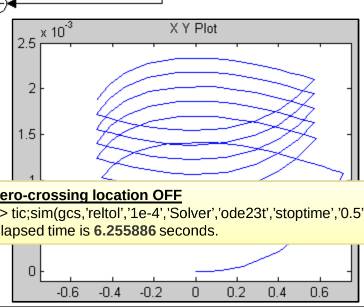


Reduced simulation time for ode23t



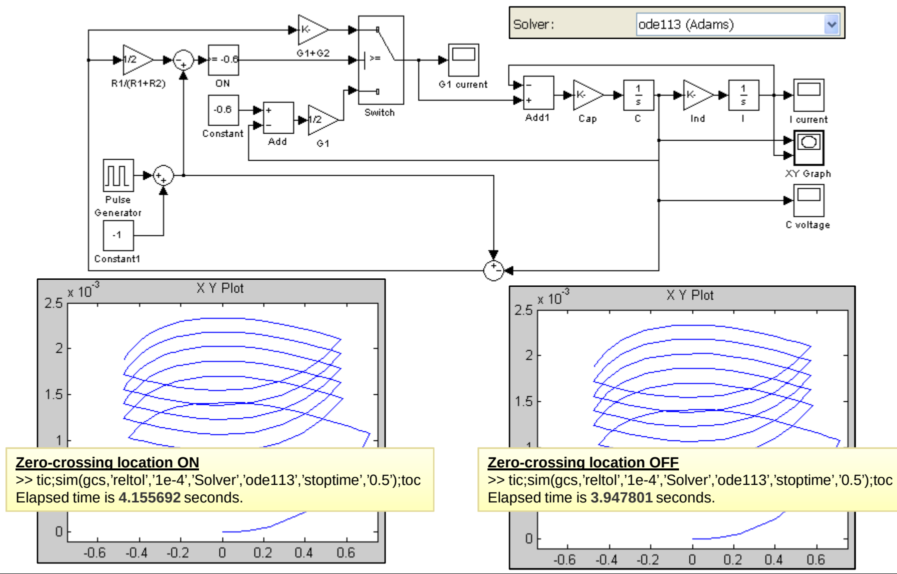


Zero-crossing location ON
>> tic;sim(gcs,'reltol','1e-4','Solver','ode23t','stoptime','0.5');toc
Elapsed time is **5.634365** seconds.



Zero-crossing location OFF
>> tic;sim(gcs,'reltol','1e-4','Solver','ode23t','stoptime','0.5');toc
Elapsed time is **6.255886** seconds.

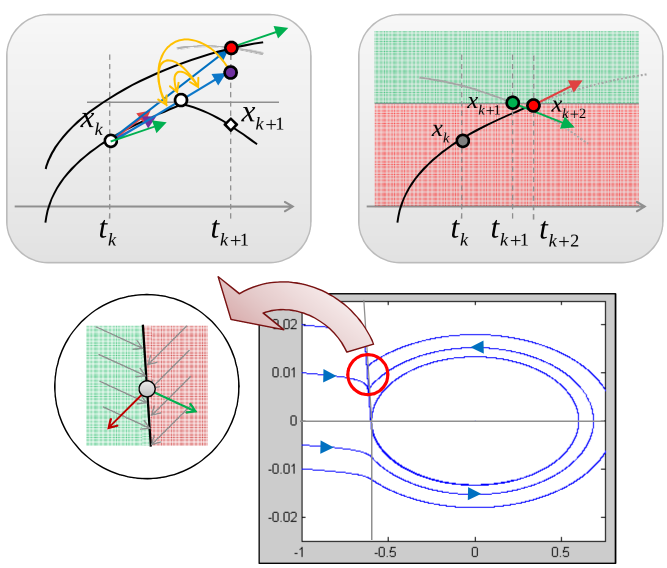
But not for ode113 … because it resets its history anyway



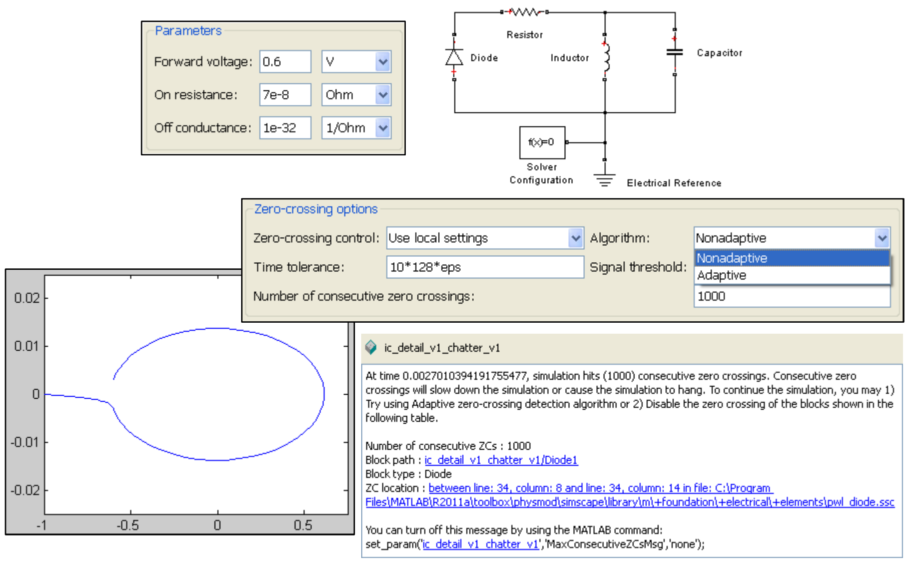
Zero-crossing location ON
>> tic;sim(gcs,'reltol','1e-4','Solver','ode113','stoptime','0.5');toc
Elapsed time is **4.155692** seconds.

Zero-crossing location OFF
>> tic;sim(gcs,'reltol','1e-4','Solver','ode113','stoptime','0.5');toc
Elapsed time is **3.947801** seconds.

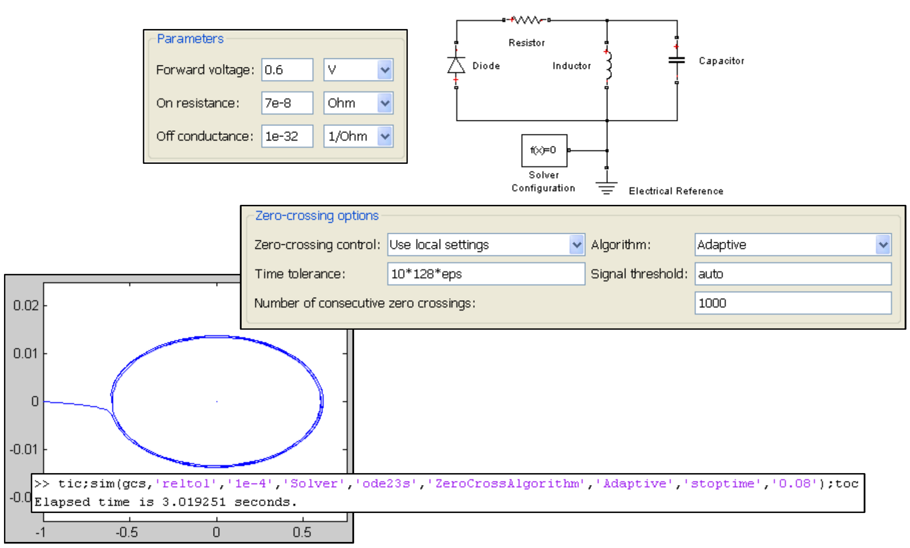
Is computational complexity the only zero crossing issue?



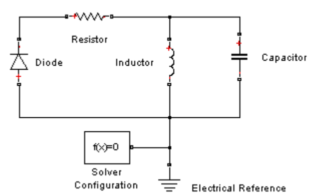
Chattering in our electrical circuit

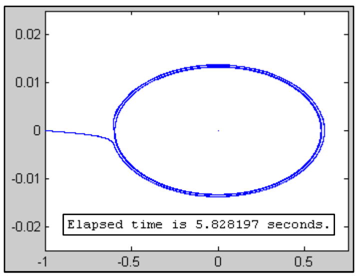


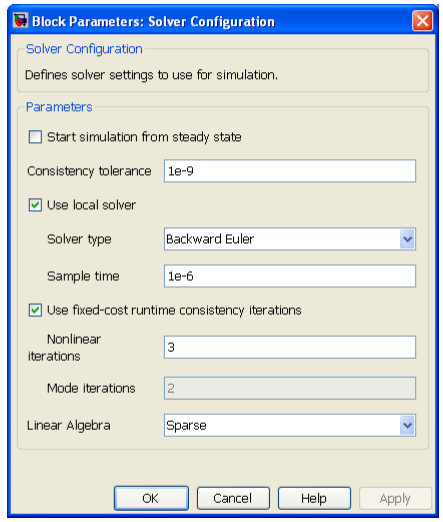
Resolve the chattering by adaptive zero crossings



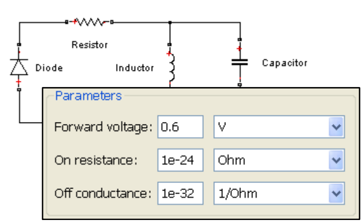
Or, employ a Simscape fixed-step solver with fixed cost

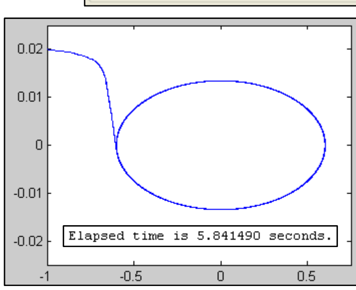


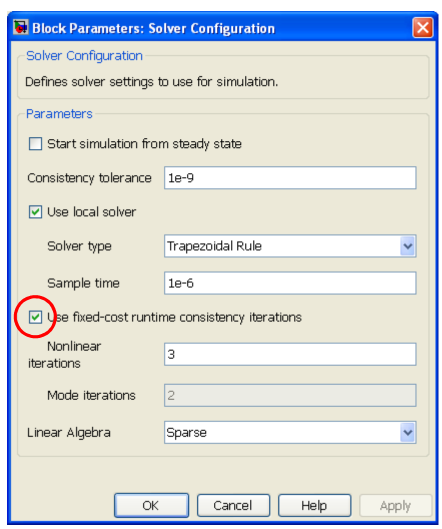




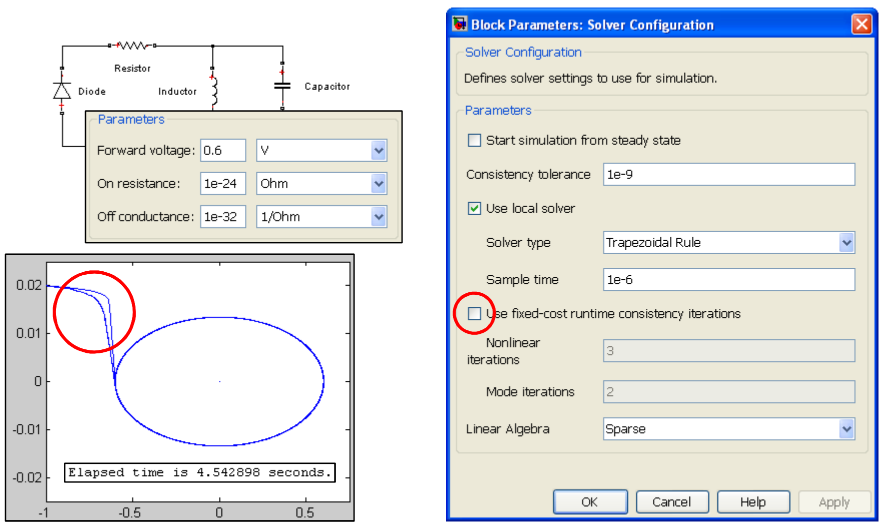
But a fixed-cost solver may be less accurate







But a fixed-cost solver may be less accurate



Agenda

- Constructing models with increasing fidelity
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  - Fixed step solver methods
  - Variable step solver methods
  - Zero crossings
- Conclusions

Conclusions

- Solvers selection is a trade off
  - Stability
  - Accuracy
  - Time to simulate
- Compare different solvers and solver parameters
  - Use a computationally expensive variable-step solver to generate a reference solution
  - If the model is sensitive, investigate why

Characterization

- My model
  - Must have a predictable execution time (could be long)
  - Must have a short simulation time
  - Has widely varying time constants (stiff)
  - Includes discontinuities
  - Includes many discontinuities
  - Exhibits chattering
  - Should not be dissipative
- My solver
  - Fixed step vs. variable step
  - Explicit vs. implicit
  - Single step vs. multi step
  - Zero crossing location or not

NB: Fixed step solvers do not do root finding

Characterization

- My model
  - Must have a predictable execution time (could be long)
  - Must have a short simulation time
  - Has widely varying time constants (stiff)
  - Includes discontinuities
  - Includes many discontinuities
  - Exhibits chattering
  - Should not be dissipative
- My solver
  - Fixed-step integration
    - Experiment with integration order, step size, and accuracy

Characterization

- My model
  - Must have a predictable execution time (could be long)
  - Must have a short simulation time
  - Has widely varying time constants (stiff)
  - Includes discontinuities
  - Includes many discontinuities
  - Exhibits chattering
  - Should not be dissipative
- My solver
  - Fixed-step integration
    - If the accuracy suffices
  - Variable-step integration
    - Multi-step methods are preferred
    - Zero-crossing on may shorten simulation time

Characterization

- My model
  - Must have a predictable execution time (could be long)
  - Must have a short simulation time
  - Has widely varying time constants (stiff)
  - Includes discontinuities
  - Includes many discontinuities
  - Exhibits chattering
  - Should not be dissipative
- My solver
  - Preferably implicit
  - Fixed step
    - ode14x
  - Variable step
    - ode15s, ode23s, ode23t, ode23tb

Characterization

- My model
  - Must have a predictable execution time (could be long)
  - Must have a short simulation time
  - Has widely varying time constants (stiff)
  - Includes discontinuities
  - Includes many discontinuities
  - Exhibits chattering
  - Should not be dissipative
- My solver
  - Variable-step integration
    - No integration history (at least single step) with zero crossing location
    - ode23t

Characterization

- My model
  - Must have a predictable execution time (could be long)
  - Must have a short simulation time
  - Has widely varying time constants (stiff)
  - Includes discontinuities
  - Includes many discontinuities
  - Exhibits chattering
  - Should not be dissipative
- My solver
  - Fixed-step integration
    - If the accuracy suffices
    - Choose the fundamental sample time as the step size

Characterization

- My model
  - Must have a predictable execution time (could be long)
  - Must have a short simulation time
  - Has widely varying time constants (stiff)
  - Includes discontinuities
  - Includes many discontinuities
  - Exhibits chattering
  - Should not be dissipative
- My solver
  - Fixed-step integration
    - If the accuracy suffices
  - Variable-step integration
    - Adaptive zero crossing location

Characterization

- My model
  - Must have a predictable execution time (could be long)
  - Must have a short simulation time
  - Has widely varying time constants (stiff)
  - Includes discontinuities
  - Includes many discontinuities
  - Exhibits chattering
  - Should not be dissipative
- My solver
  - Nondissipative integration method
    - ode23t

And …

Do not fall in love with a model ☺

-- Jacques LeFèvre

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