



# Initial Condition Strategies for Multiple-time Partial Differential Equations

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# Collaborators

-  team at Sandia
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# What are MPDEs?

- Multi-time Partial Differential Equations
- An approach for faster simulation of oscillatory DAEs
- Convert an ODE/DAE into a multi-time PDE/PDAE
- Introduce new time variable as a spatial variable
- Savings come from periodicity of new time variable
- Can recover ODE/DAE solution from MPDE solution
- Motivation: Speedups of 100x to 1000x!

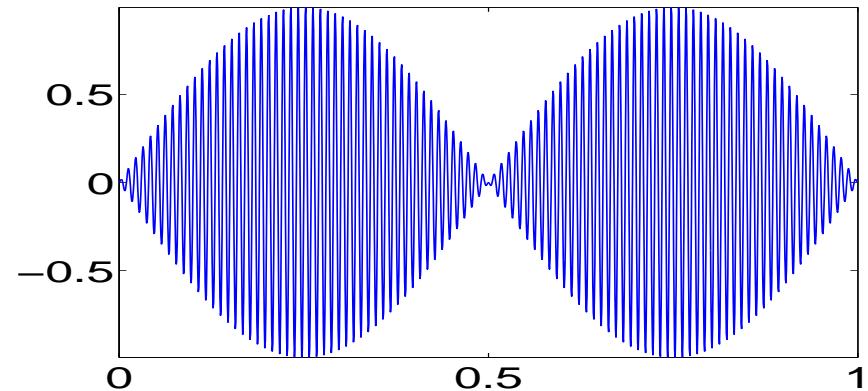
# Representation of multi-rate signals

- $b(t) = \sin(2\pi t) \sin(2\pi 10^2 t)$

arclength  $\approx 254.7$

15 points / 4.2 arclength

$\approx 910$  samples

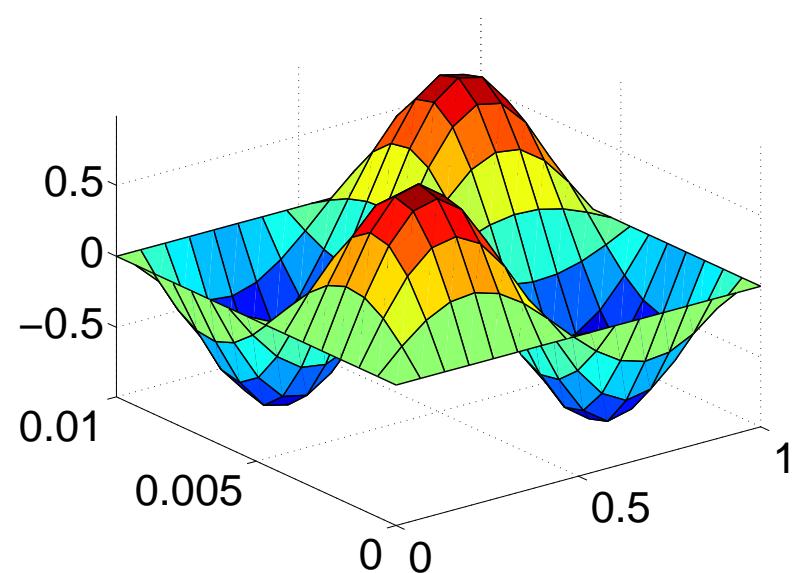


- $\hat{b}(t_1, t_2) = \sin(2\pi t_1) \sin(2\pi 10^2 t_2), \quad b(t) = \hat{b}(t, t)$

$t_1$  arclength  $\approx 4.2$

$t_2$  arclength  $\approx 4.2$

$\approx 225$  samples



# Research Context

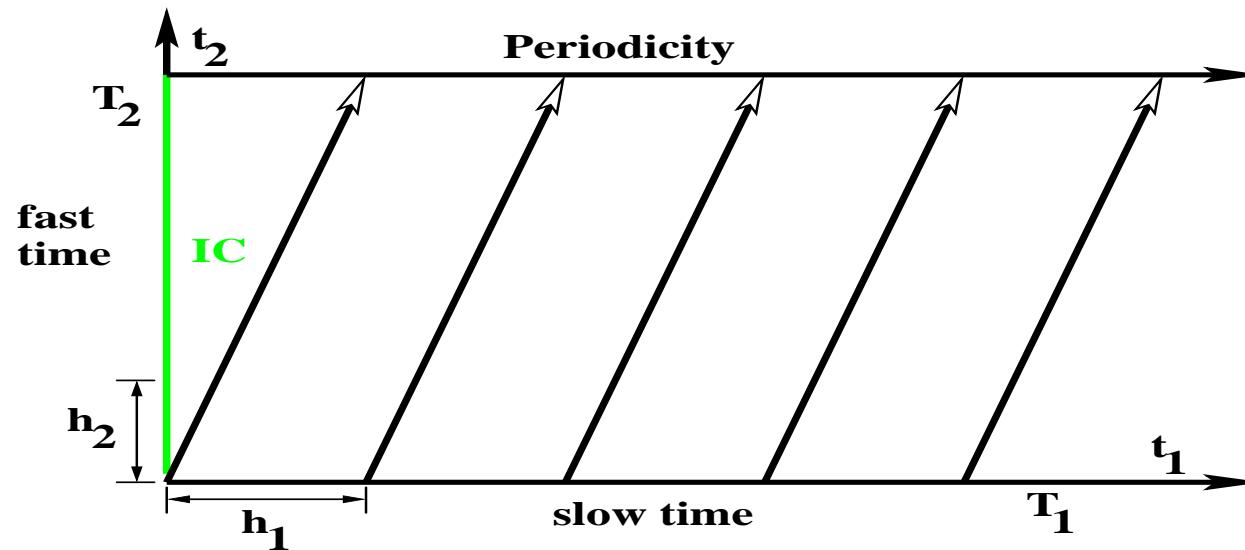
- Time-domain envelope methods:
  - L. Petzold 1981
  - K. Kundert et al. 1988
- Frequency-domain envelope methods:
  - E. Ngoya / R. Larchevéque 1996
  - D. Sharrit 1996
  - P. Feldmann / J. Roychowdhury 1996
- Time and frequency domain MPDE methods:
  - H-G. Brachtendorf et al. 1996
  - J. Roychowdhury 2001
  - Fourier envelope robustness: J. Roychowdhury 2002
  - Discretization: Coffey, Roychowdhury, et al 2004

# Circuit transformation

- Re-write circuit DAE using multi-time variables
  - DAE:  $\frac{d\mathbf{q}(\mathbf{x})}{dt} + \mathbf{f}(\mathbf{x}) + \mathbf{b}(t) = 0$
  - MPDE:  $\frac{\partial \mathbf{q}(\hat{\mathbf{x}})}{\partial t_1} + \frac{\partial \mathbf{q}(\hat{\mathbf{x}})}{\partial t_2} + \mathbf{f}(\hat{\mathbf{x}}) + \hat{\mathbf{b}}(t_1, t_2) = 0$
- $\hat{\mathbf{x}}(t_1, t_2)$  = vector of multi-time unknowns
- $\hat{\mathbf{b}}(t_1, t_2)$  = multi-time input
- Solution of MPDE  $\implies$  solution of DAE
  - $\hat{\mathbf{b}}(t, t) = \mathbf{b}(t) \implies \mathbf{x}(t) = \hat{\mathbf{x}}(t, t)$
- Solve multi-time formulation directly

# Efficiency

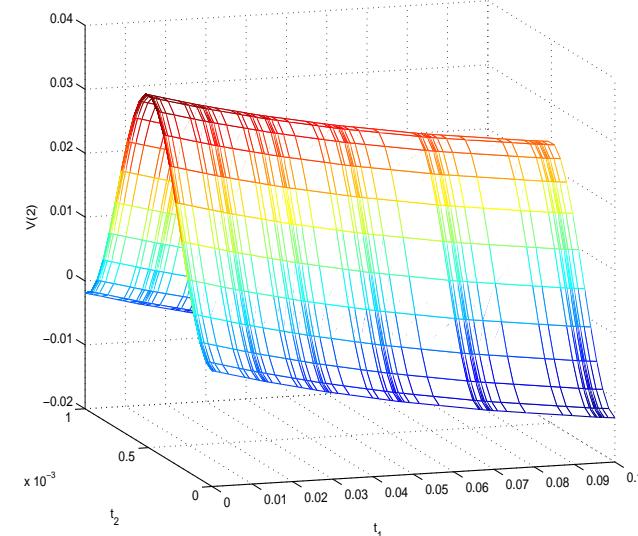
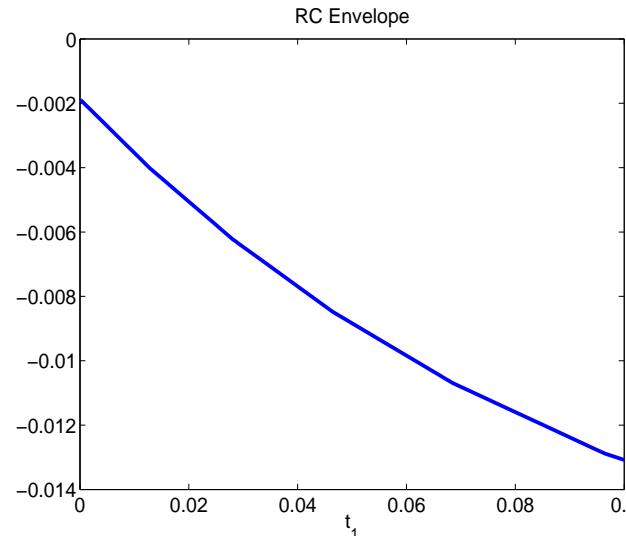
- We've turned a DAE into a 2-D PDAE
- Quasi-periodicity of fast oscillation



- Frequency gap between rates of change:  
Need at least 100x difference for 2-D MPDE

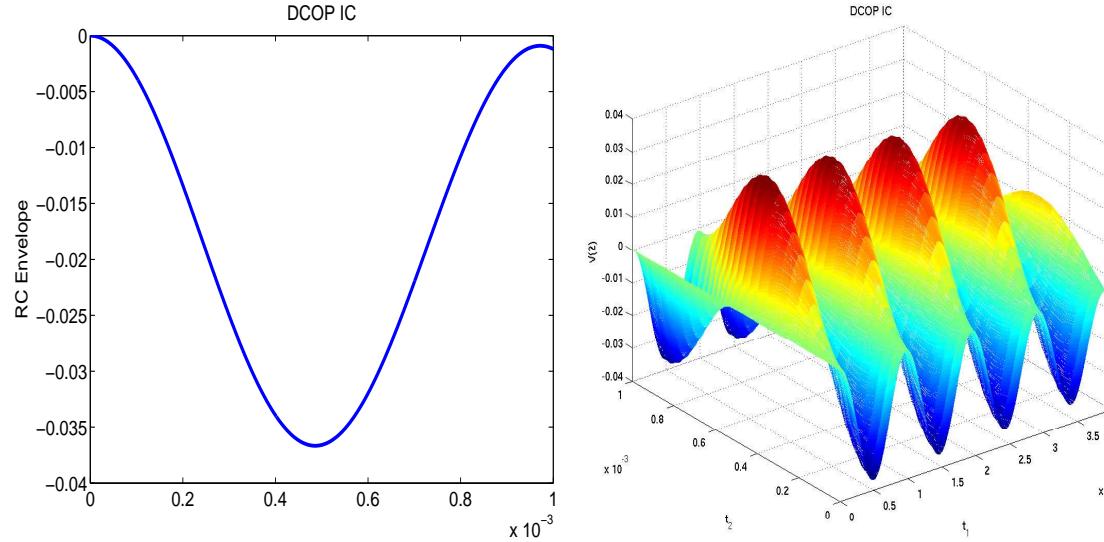
# Initial Condition Strategies

- Five strategies
  - Basic explanation
  - Pro & Con
1. DCOP
  2. Integrate
  3. Integrate & Interpolate
  4. Steady state with slope
  5. Optimization

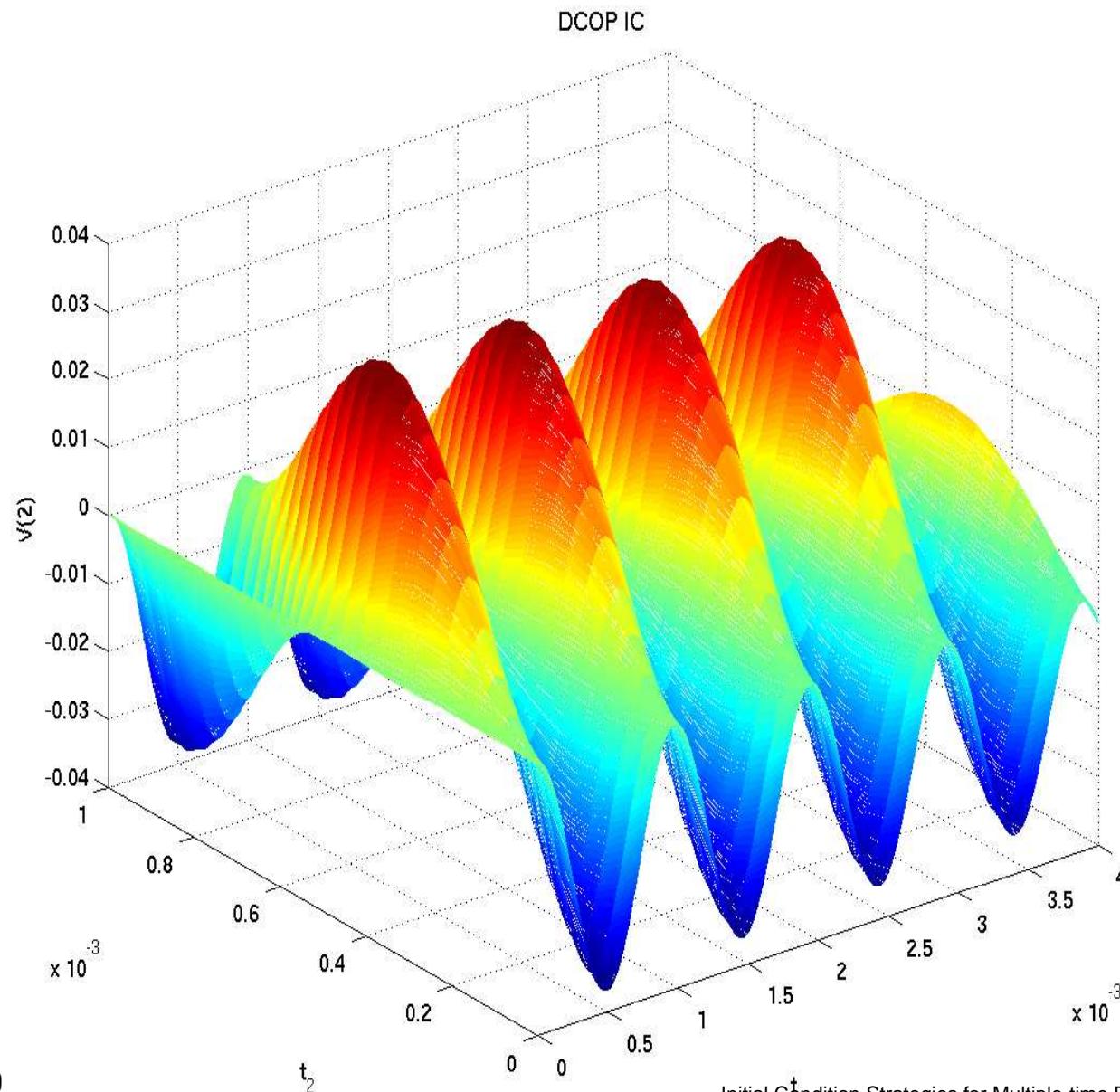


# IC 1: DCOP

- DCOP: DC Operating Point  
Consistent initial condition for DAE problem
- Pro: Free, periodic
- Con: Does not represent oscillations

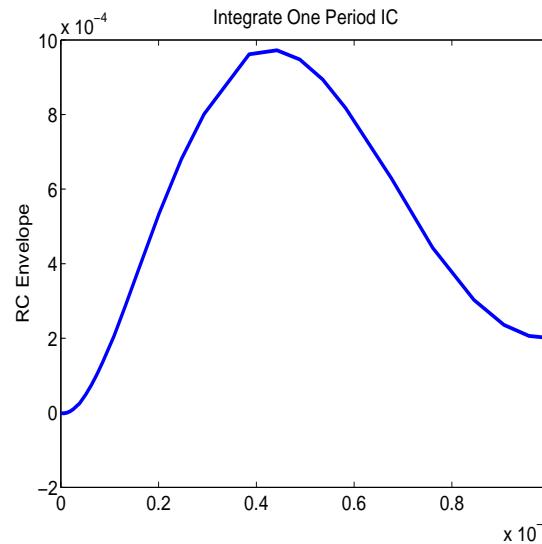


# IC 1: DCOP IC MPDE output



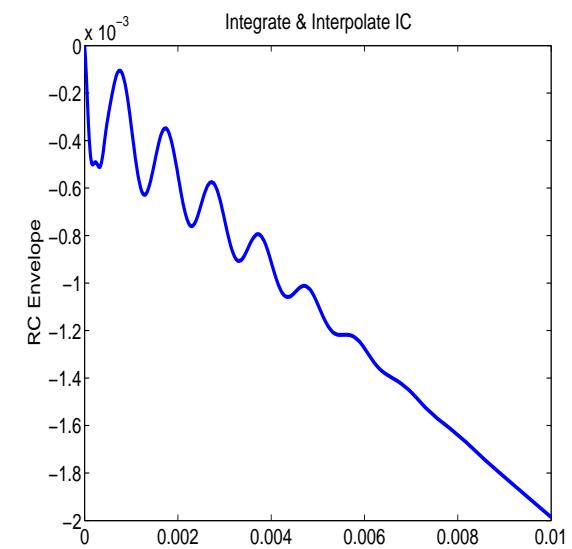
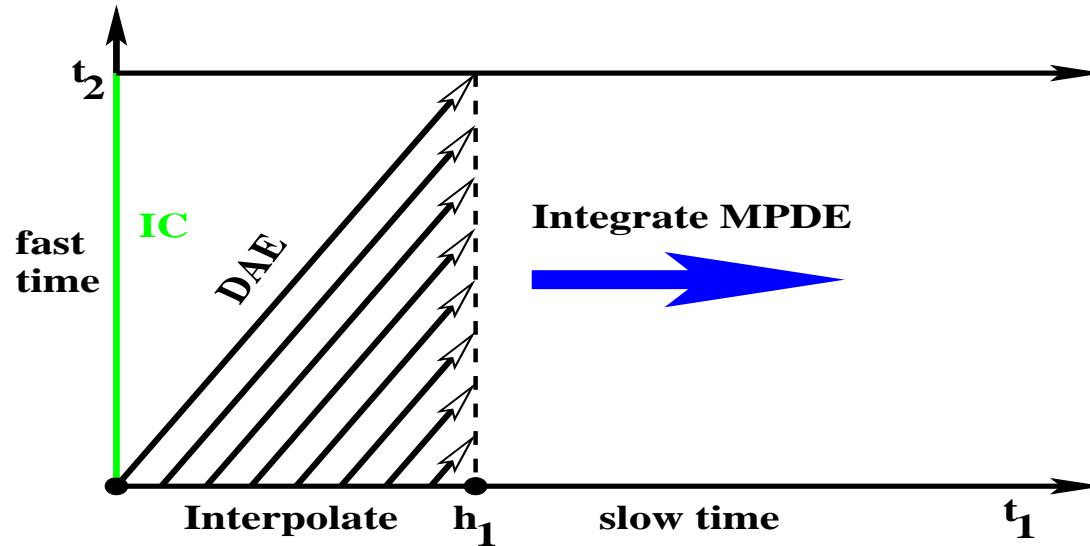
# IC 2: Integrate one fast period

- Integrate one fast period as MPDE IC
- Pro: low cost: 1 period
- Con: not periodic



# IC 3: Integrate & Interpolate

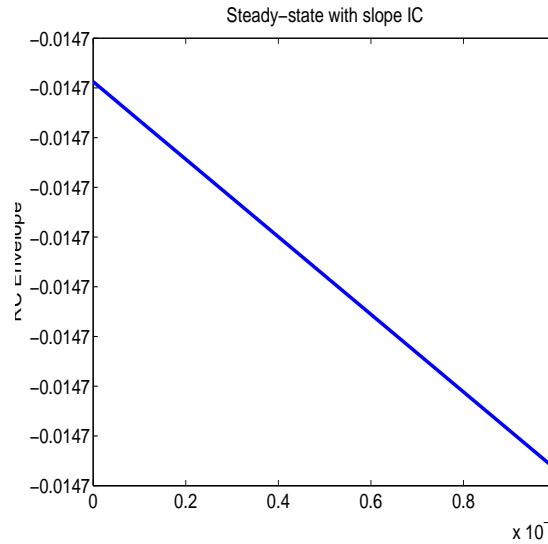
- Integrate DAE one fast period then interpolate to form new DAE IC for integrating to MPDE IC



- Pro: periodic
- Con: cost:  $(n_2 + 1)/2$  periods

# IC 4: Steady-state with Slope

- Integrate one period to estimate  $\frac{\partial \mathbf{q}(\hat{\mathbf{x}})}{\partial t_1} = \gamma$
- Solve for  $\hat{\mathbf{x}}(0, t_2)$ :  $\gamma + \frac{\partial \mathbf{q}(\hat{\mathbf{x}})}{\partial t_2} + \mathbf{f}(\hat{\mathbf{x}}) + \hat{\mathbf{b}}(0, t_2) = 0$
- Pro: fairly cheap: 1 period + nonlinear solve, fast source oscillations well represented
- Con: IC based only at  $t_1 = 0$



# IC 5: Optimization

- Consider the simplified MPDE problem:

$$\begin{aligned}\frac{\partial \hat{\mathbf{x}}}{\partial t_1} + \frac{\partial \hat{\mathbf{x}}}{\partial t_2} + \mathbf{f}(\hat{\mathbf{x}}) + \hat{\mathbf{b}}(t_1, t_2) &= 0 \\ \hat{\mathbf{x}}(0, t_2) &= \mathbf{v}(t_2), \quad \mathbf{v}(0) = x_0\end{aligned}$$

- Formulate unconstrained minimization problem

$$\min_{v \in U} |J(v) - \gamma|, \quad J(v) = \frac{1}{2} \int_0^T \int_0^T \left| \frac{\partial \hat{\mathbf{x}}}{\partial t_1} \right|^2 dt_1 dt_2$$

- Pro: periodic, increase step-sizes
- Con: high cost:  $2n_2$  periods/iteration

# Optim: Related ODE problem

- Assume  $\hat{\mathbf{b}}(t_1, t_2) = \mathbf{b}(t_2)$   
The sources produce only fast oscillations
- This produces the following related problem:

$$\dot{\mathbf{x}} + \mathbf{f}(\mathbf{x}) + \mathbf{b}(t + s) = 0, \quad \mathbf{x}(0; s) = \mathbf{v}(s)$$

- $\hat{\mathbf{x}}(t_1, t_2) = \begin{cases} \mathbf{x}(t_1, t_2 - t_1), & t_2 > t_1 \\ \mathbf{x}(t_1, t_2 - t_1 + T), & t_2 < t_1 \end{cases}$
- We can compute MPDE solutions by solving a perturbed ODE problem
- Transform our objective function:

$$J(\mathbf{v}) = \frac{1}{2} \int_0^T \int_0^T |\dot{\mathbf{x}}(t; s) - \mathbf{x}_s(t; s)|^2 dt ds$$



# Optim: Gradient & adjoint equations

- The gradient is a function  $s \mapsto g$  given by:

$$g = p(0; s) - \dot{x}(0; s) + x_s(0; s), \quad s \in (0, T)$$

- where  $p = p(t; s)$  is computed by solving the adjoint equations:

$$-\dot{p} + \left( \frac{\partial f}{\partial x} \right)^T p + \left( \frac{d}{dt} - \frac{d}{ds} \right) x(t; s) = 0$$

$$p(T; s) = \dot{x}(T; s) - x_s(T; s)$$

- We have continuous & discrete analysis for fully nonlinear DAE case

# Optim: Steps for gradient

Recall gradient and adjoint equations:

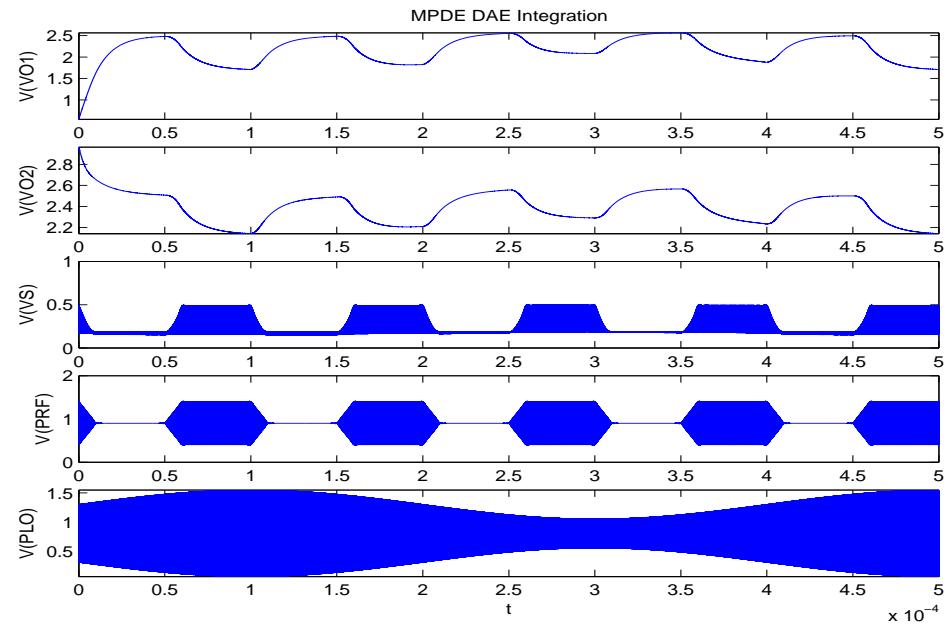
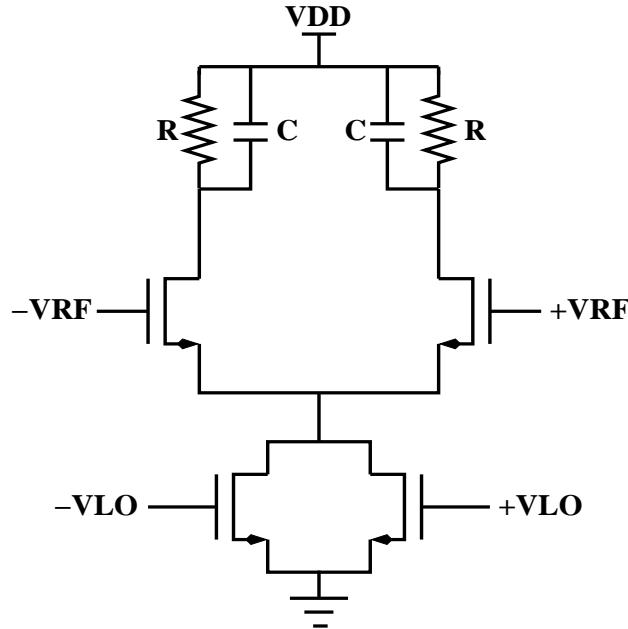
$$\begin{aligned} \mathbf{g}(s) &= \mathbf{p}(0; s) - \dot{\mathbf{x}}(0; s) + \mathbf{x}_s(0; s) \quad \text{for } s \in (0, T) \\ -\dot{\mathbf{p}} + \left(\frac{\partial \mathbf{f}}{\partial \mathbf{x}}\right)^T \mathbf{p} + \left(\frac{d}{dt} - \frac{d}{ds}\right) \mathbf{x}(t; s) &= 0 \\ \mathbf{p}(T; s) &= \dot{\mathbf{x}}(T; s) - \mathbf{x}_s(T; s) \end{aligned}$$

- Specify  $\mathbf{v}$  as input
- Solve forward problem for  $\mathbf{x}(t; s)$ ,  $\forall s \in (0, T)$
- Form  $J(\mathbf{v})$
- Solve adjoint equations for  $\mathbf{p}(0; s)$ ,  $\forall s \in (0, T)$
- Form gradient  $\mathbf{g}(s)$



# Communication Speed-up Example

- Balanced CMOS direct-downconversion mixer



- Sources:
  - $+VLO = 450\text{Mhz}$  sinusoid modulated by  $2.4\text{khz}$  sinusoid
  - $+VRF = 900\text{Mhz}$  carrier modulated by  $10\text{kbps}$  bitstream
- DAE simulation time:  $\approx 5$  days

# IC Performance

Communication Example Circuit (time in min)

	IC Time	MPDE Time	Total
DCOP	N/A	N/A	N/A
Integrate & Interpolate	5.2	18.3	23.5
Integrate	0.08	12.3	12.4
Steady state w/slope	0.12	13.1	13.2
Optimization	14.0	11.4	25.4
DAE			$\approx 7600$

Note  $\approx 600x$  speed-up!

# Conclusions

- MPDE methods offer considerable speed-up
- Choice of IC is very important:  
Optimization may be helpful, but it needs to be cheap.
  - Interesting application of adjoint equation theory
  - Improves accuracy & speed-up
  - Captures some start-up behavior
- Fast time axis must represent oscillation well to get speedup

Thank you!

