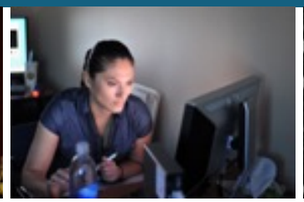
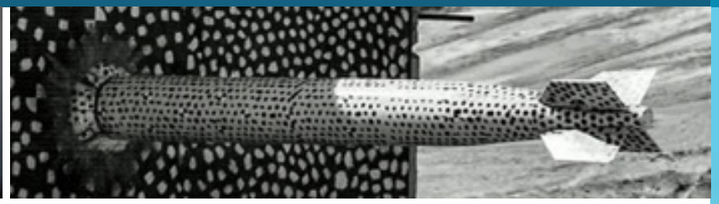
Enabling Scalable Predictive Circuit Simulation using Trilinos





PRESENTED BY

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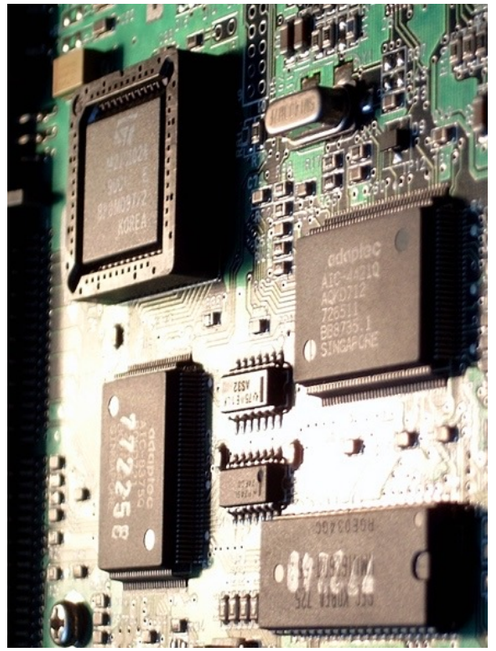
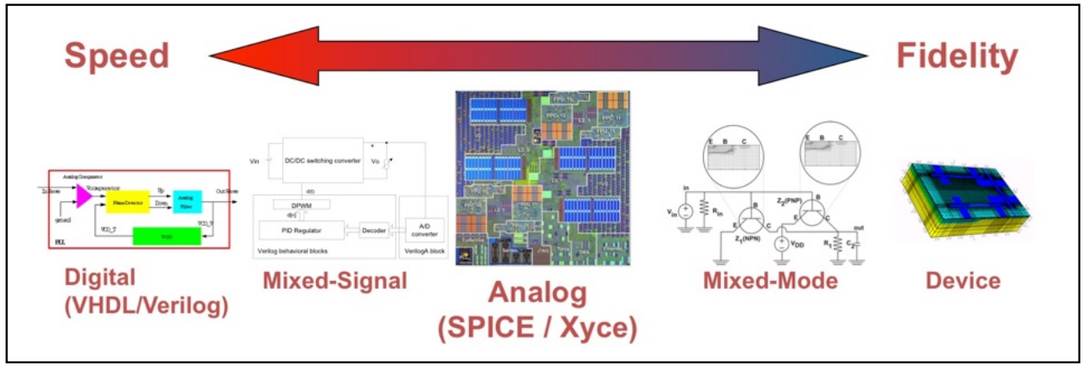
Outline

- What is circuit simulation?
- Xyce software architecture
  - Trilinos solver stack
  - Tpetra transition effort
- Highlights of capabilities and performance
  - Linear solver development
  - Recent solver improvements



What is circuit simulation?

Definition: A technique for checking and verifying the design of electrical and electronic circuits and systems prior to manufacture and deployment[1]



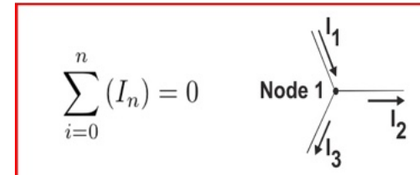
Analog circuit simulation provides tradeoff between fidelity and speed

- Models network(s) of devices coupled via Kirchoff's current and voltage laws

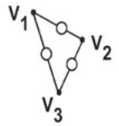
$$f(x(t)) + \frac{dq(x(t))}{dt} = b(t)$$

- SPICE[2] is the defacto industry standard for analog circuit simulation

$$\sum_{i=0}^{n} (I_n) = 0$$



$$\sum_{i=0}^{n} (\Delta V) = 0$$



○ = Device
• = Node

$$G = \frac{\delta I}{\delta V} = \text{conductance} = \text{Jacobian term}$$

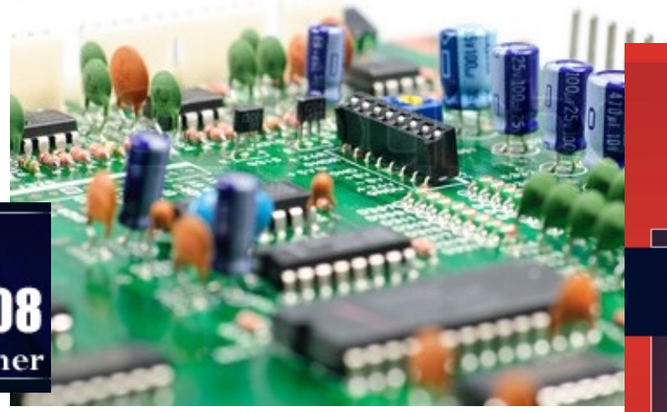
Ohm's Law: $I = GV = V/R$

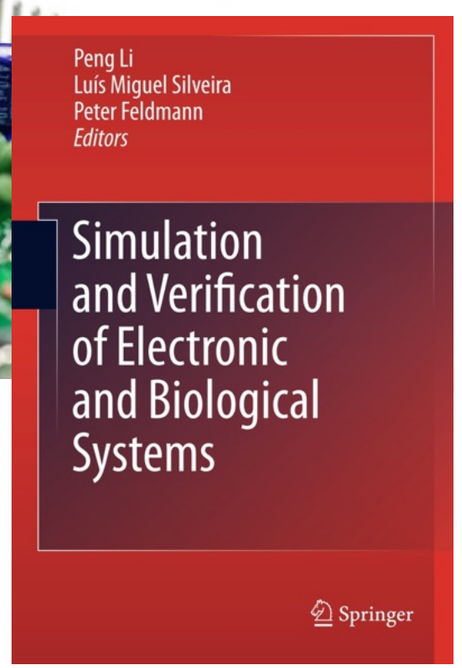
[1] Najm, F. N. Circuit Simulation. John Wiley & Sons, Inc., 2010.
[2] Nagel, Laurence W. SPICE2: A Computer Program to Simulate Semiconductor Circuits, California Univ Berkeley Electronics Research Lab, 1975.

Motivation for Xyce

Xyce provides a capability to analyze general network systems and has been integral to modeling and simulating Sandia's Complementary Metal-Oxide-Semiconductor (CMOS) circuit designs, as well as:

- Biological networks
- Neural networks
- Power grids





Single code base that efficiently and seamlessly simulates systems that can have a wide range of dynamics, topological complexity, and size (10-10^7)

- Provides support for both serial and distributed-memory parallel builds
- Open source, GPLv3, see https://xyce.sandia.gov or https://github.com/xyce

Xyce™ PARALLEL ELECTRONIC SIMULATOR

A high-level view of the Xyce simulation flow

Parsing

- Convert netlist file syntax to equivalent devices and network/circuit connectivity
- Distribute devices over multiple processors
- Determine global ordering and communication

Device Evaluation

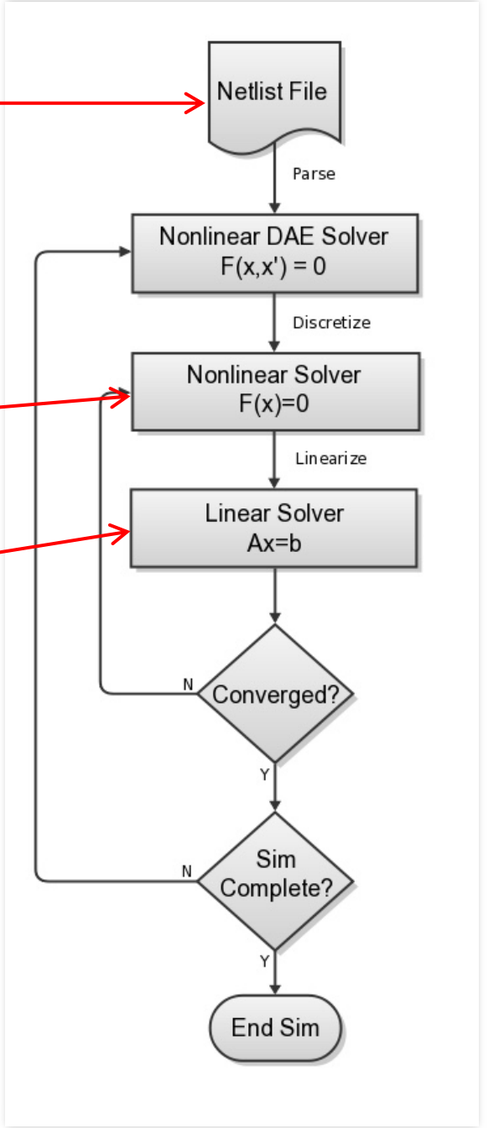
- Loop through all devices for state evaluation and matrix loading

Linear Solve

- Sparse linear algebra and solvers used to solve linearized system

Advanced Analysis Methods

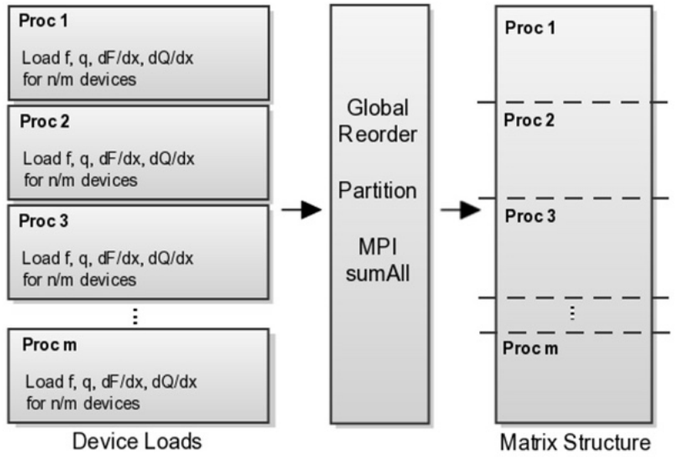
- Sampling: Monte Carlo / LHS (DAKOTA),
- Sensitivity: PCE (Stokhos)
- Optimization: ROL

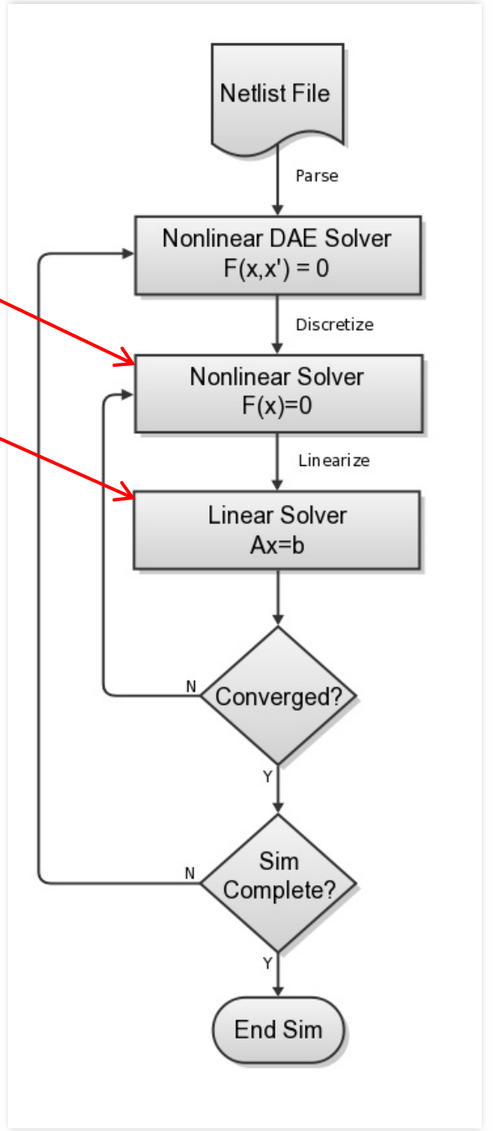


Challenges for the Xyce simulation flow

Computational load balancing

- For **smaller** circuits, performing the device evaluations dominates the total simulation time
- For **larger** circuits, solving the linear system of equations dominates the total simulation time
- A redistribution layer is employed for parallel execution to enable separate load balancing strategies

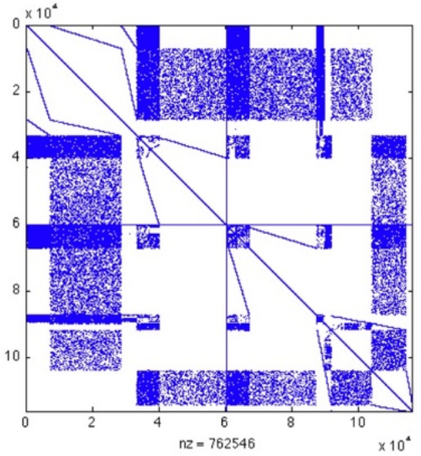


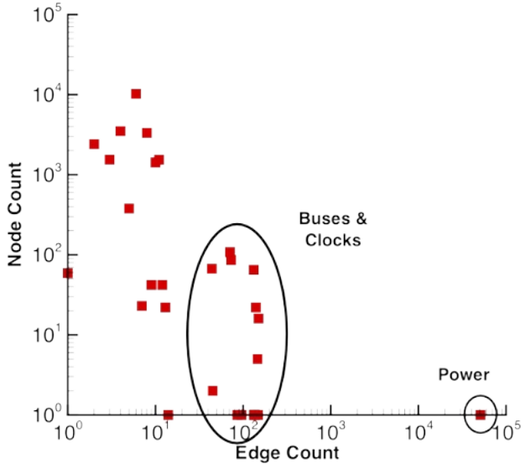


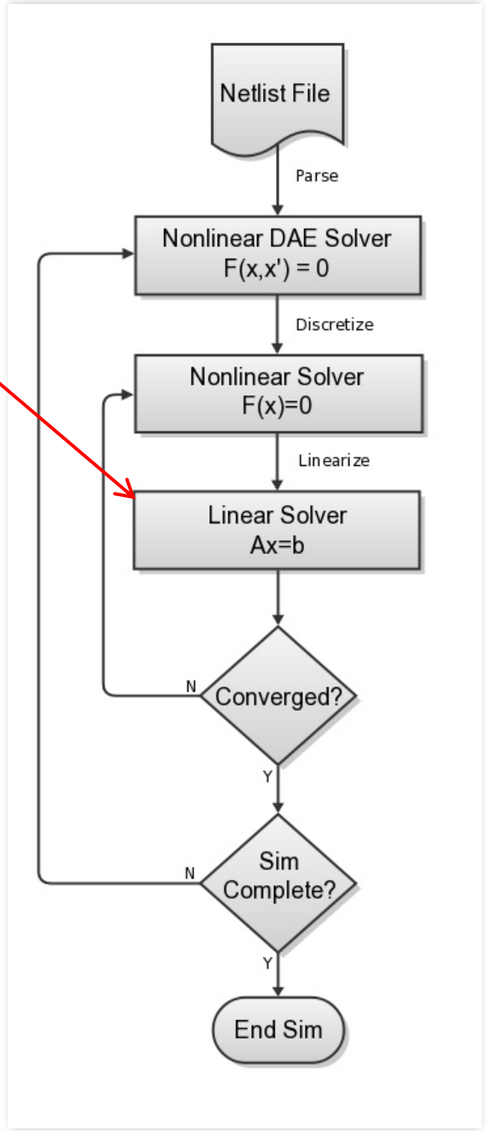
Challenges for the Xyce simulation flow

Hierarchical connectivity:

- Analog circuit simulation often generates graph structures that are hierarchical when compared to the spatial topology of PDEs
- High-connectivity nodes result in high communication in parallel execution, so removing them is beneficial
- Linear systems are predominately non-Hermitian and very sparse. Iterative solvers provide scalability, but direct solvers provide robustness

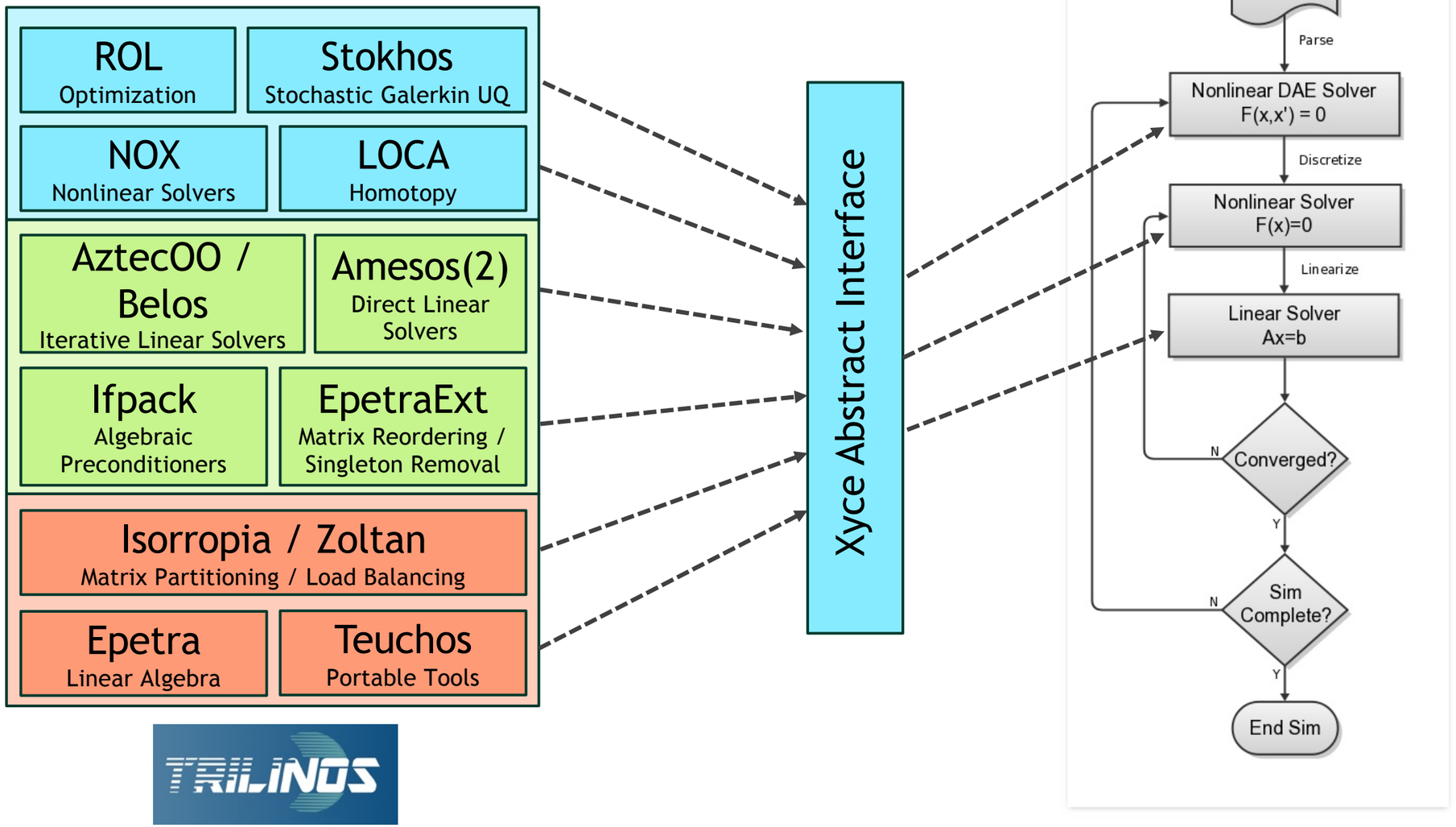




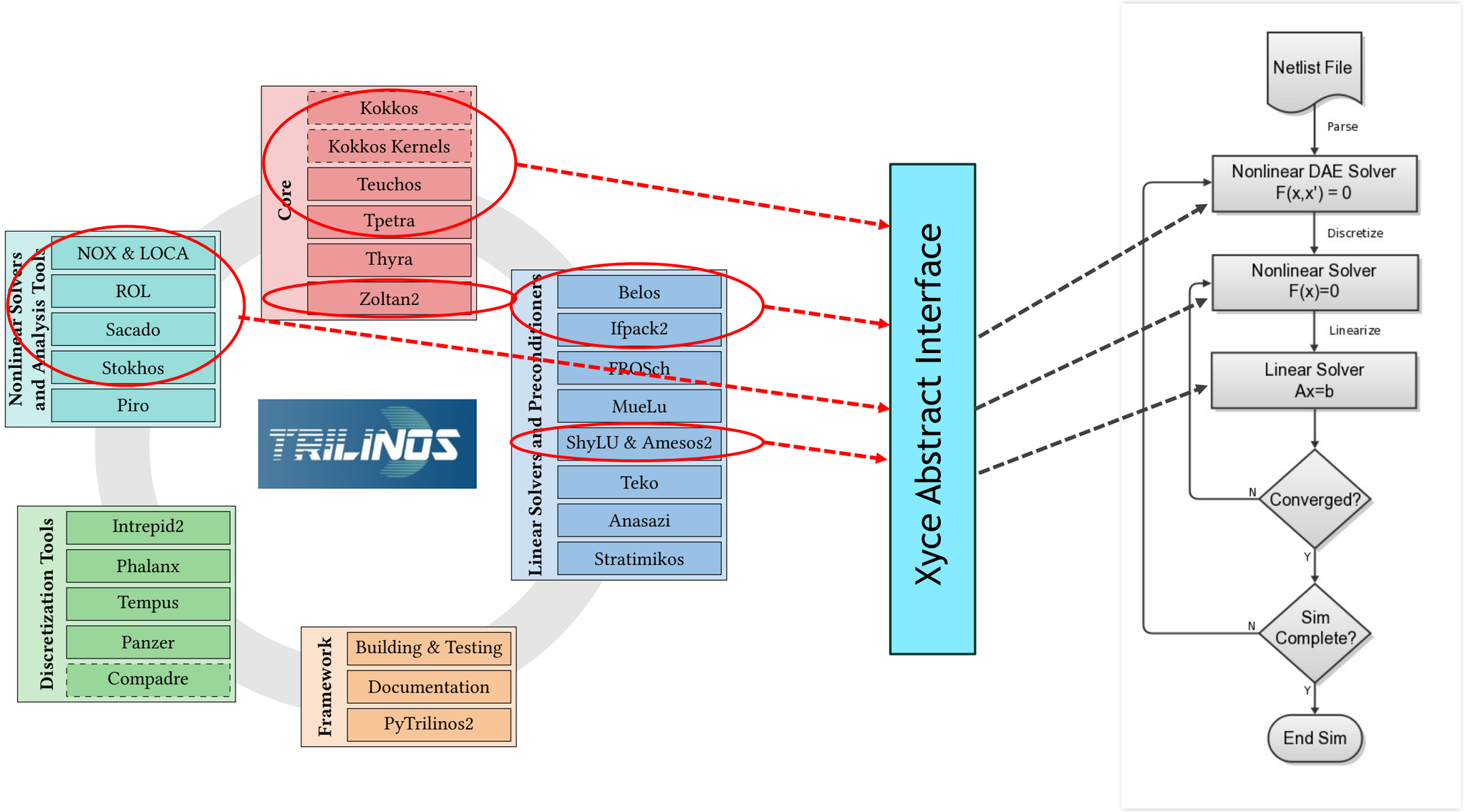


Xyce Simulation Flow + Trilinos Solver Stack

[Epetra based]



Xyce Simulation Flow + Trilinos Solver Stack
[Tpetra based]



Trilinos image courtesy of "Trilinos: Enabling Scientific Computing Across Diverse Hardware Architectures at Scale," Mayr, et al., https://arxiv.org/abs/2503.08126

Tpetra Transition Effort

Initially (circa 1999), Xyce was one of the first application codes at Sandia to fully integrate the Trilinos solver stack, which influenced its design:

- In general, Xyce abstract interfaces look a lot like Epetra
- Rampant use of raw pointers, followed by an inelegant use of smart pointers
- Direct access to matrix/vector memory in device models
- Ubiquitous use of copy semantics, instead of view, for map/graph objects, for example:

```
epetraGraph_ = Teuchos::rcp( new Epetra_CrsGraph( Copy, *epetraMap, numIndicesPerRow.data() ) );
```

- Unnecessarily leverages dynamic creation of graph/matrix objects
- Relies on supporting tools provided by EpetraExt
  - Singleton filtering
  - Partitioning interfaces
  - Remapping utilities

Tpetra Transition Effort

As Xyce was transitioning to Tpetra there were some helpful things:

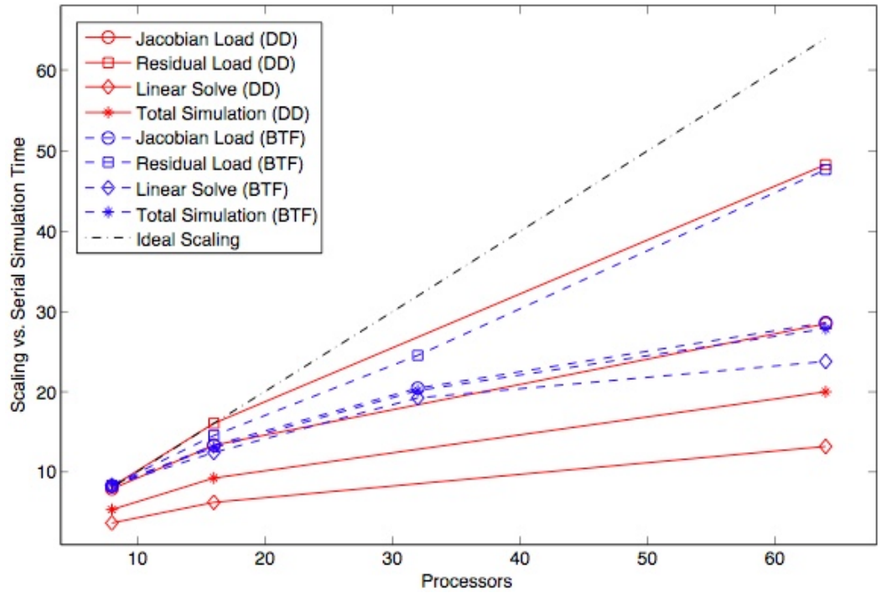
- Many of the linear algebra classes have included Epetra-esque interfaces.

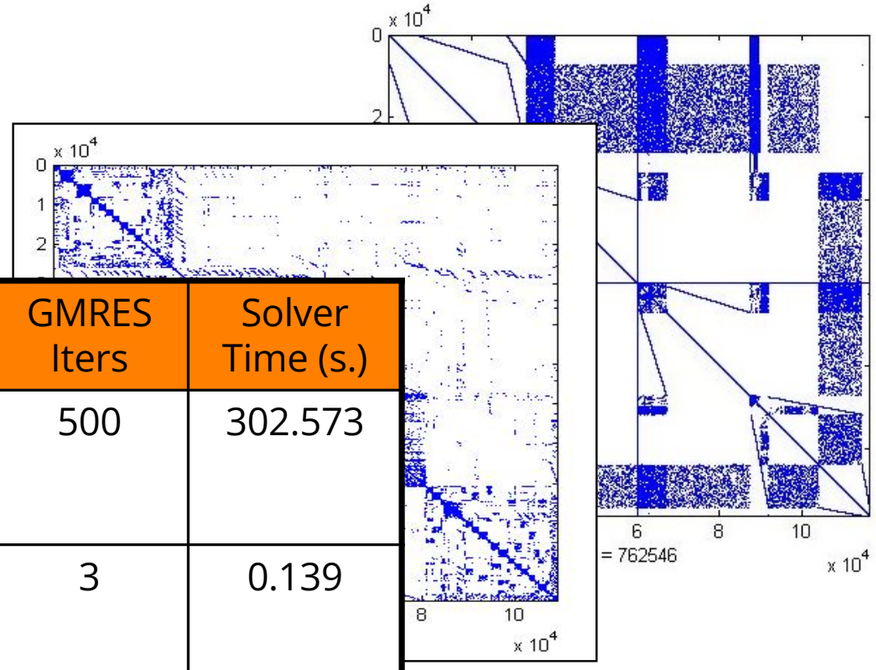
As well as some unexpected challenges:

- The need to integrate `resumeFill()` into matrix loading, particularly in cases when matrix loading is a multi-stage process
- Obtaining a pointer to underlying memory to pass to the device models required interacting with Kokkos objects, often disguised by a typedef
- Some capabilities required by block analysis methods may not be compatible with Tpetra design
- Non-member helper functions were introduced to provide “all-in-one” methods to create new objects by import/export data, but the results were mixed

Trilinos supports linear solver development for Xyce

- **Custom approaches for linear solvers have been necessary to achieve scalable performance for analog simulation**
- For small scale circuits, the Dulmage-Mendelsohn permutation (BTF) was leveraged in the KLU sparse direct solver [Tim Davis (UF, Texas A&M)]
- BTF structure was leveraged to create a new preconditioned iterative method
  - Great for (older) CMOS memory circuits
  - Circuits with parasitics are more challenging





Preconditioning Method	Residual	GMRES Iters	Solver Time (s.)
Local AMD ILUT ParMETIS	3.43e-01 (FAIL)	500	302.573
BTF Block Jacobi Hypergraph	3.47e-10	3	0.139

Linear Solver Improvements (2016)

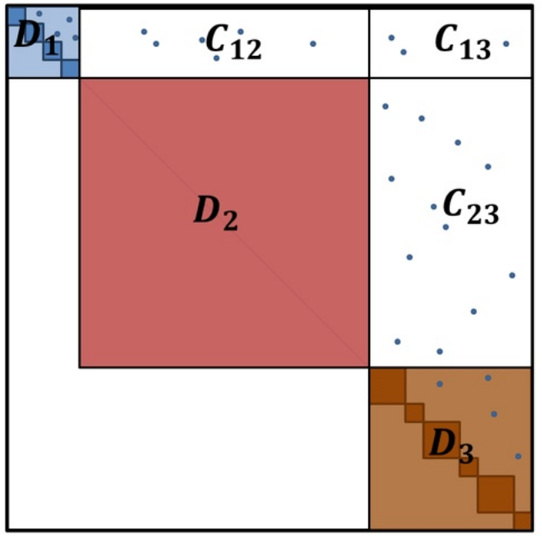
Trilinos-Amesos2: Basic sparse LU factorization with row-pivoting

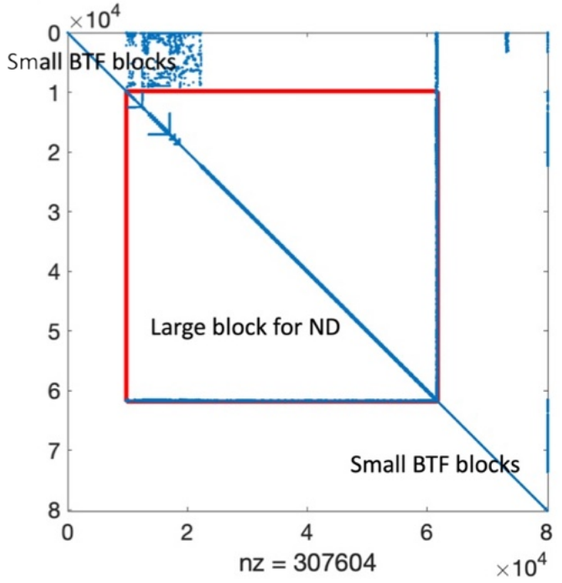
Templated on a scalar type, `BASKER_ScalarTraits<>`

- Default / Copy constructor
- Arithmetic operators: +,-,*,/
- Relational/comparison operators: ==, !=, >, <
- Multiple linear algebra (Epetra, Tpetra) adapters exist in Amesos2

Multi-threaded version (ShyLU-Basker)[3]:

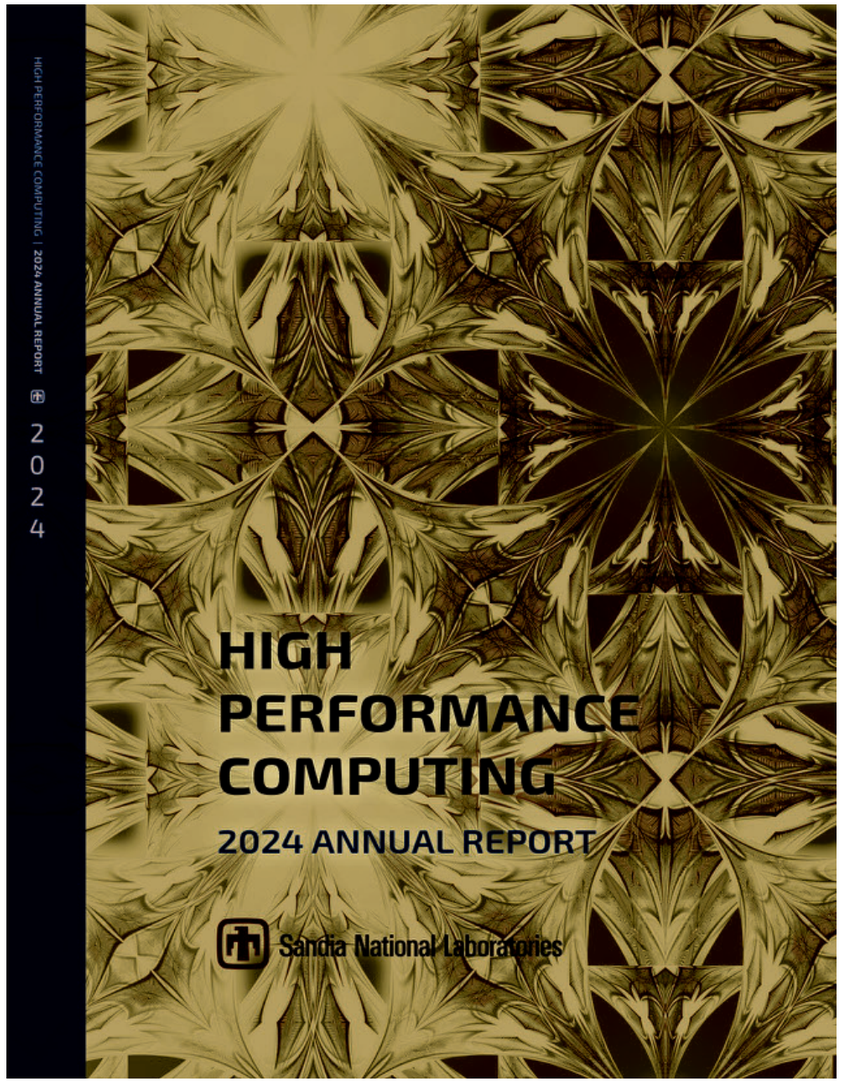
- Parallelizes the Gilbert-Peierls algorithm
- Uses hierarchical data layouts to expose fine-grain parallelism and map to memory structure of most-many core systems
  - Block triangular form (BTF) to compute coarse structure
  - Nested Dissection (ND) to expose parallelism for large diagonal blocks (ex. D_2)
- Improves transient performance in Xyce for small to medium sized circuits





[3] "Basker: A Threaded Sparse LU Factorization Utilizing Hierarchical Parallelism and Data Layouts," J. Booth, S. Rajamanickam, and H. Thornquist, 2016 IEEE IPDPSW, pp. 673-682.

Recent Solver Improvements (2024)



Radiation-aware Xyce simulations of memory circuits

Integrated circuit simulation for design

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the microelectronics community and form the basis for the electronic design automation industry.

One type of computational analysis is circuit simulation[1] and involves a

the Berkeley SPICE program,[2]

to constraints not present in analog designs, and these constraints can often be exploited to expedite computational analysis. Hence, the traditional

simulators, using standard cell models as input.

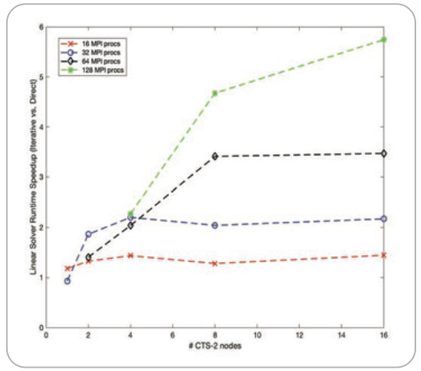


FIGURE 1

Runtime speedup of block subdomain preconditioned method (overlap = 1, Intel MKL Pardiso, 4 threads) compared to direct method (Intel MKL Pardiso, 16 threads) in simulating SRAM circuit on CTS-2. The MPI processors are varied from 16, 32, 64, and 128, while the number of CTS-2 nodes are varied from 1,2,4,8, and 16.

Trilinos-enabled frequency-domain simulation in Xyce

Harmonic Balance analysis is a frequency-domain simulation technique used to efficiently calculate the steady-state response of nonlinear RF and microwave circuits

$$\frac{dq(x)}{dt} + f(x) = b(t),$$

using Fourier series expansions for $x(t)$ and $b(t)$: $x(t) = \sum_{i=-\infty}^{\infty} X_i e^{ji\frac{2\pi}{T}t}, \quad b(t) = \sum_{i=-\infty}^{\infty} B_i e^{ji\frac{2\pi}{T}t}$

$$H_{HB} = \Omega Q(X) + F(X) - B = 0 \qquad \mathbf{\Omega} = \begin{pmatrix} -Mj\omega_0 & & \\ & \ddots & \\ & & Mj\omega_0 \end{pmatrix}, \omega_0 = \frac{2\pi}{T}$$

Expanding the frequency-domain equations using the discrete Fourier transform matrices, D and D^{-1}

$$\mathbf{H_{HB}} = \Omega D \mathbb{Q}(.) D^{-1} X + D \mathbb{F}(.) D^{-1} X - B$$

$$\mathbf{J_{HB}} = \Omega D \mathbb{C} D^{-1} + D \mathbb{G} D^{-1},$$

$$\mathbb{C} = \begin{pmatrix} C(t_0) & & \\ & \ddots & \\ & & C(t_{2M}) \end{pmatrix}, C(t_i) = \frac{dq}{dx}|_{x(t_i)} \qquad \mathbb{G} = \begin{pmatrix} G(t_0) & & \\ & \ddots & \\ & & G(t_{2M}) \end{pmatrix}, G(t_i) = \frac{df}{dx}|_{x(t_i)}$$

Linear Solver Improvements (2017)

Harmonic Balance linear solvers for the block-structured Jacobian matrix are challenging to develop

- Large matrix (n x N) with block structure, complex-valued, dense blocks
- Iterative methods are most often used because they avoid Jacobian matrix construction
  - For highly-nonlinear circuits effective preconditioners are difficult to construct
  - Preconditioners for linear to mildly-nonlinear circuits have been implemented in Xyce

A direct solver was developed using the templated Basker direct solver in Amesos2

- Enables the use of “block matrices” as a scalar type
- Motivated by the Berkeley Design Automation (BDA) direct solver[4]
- **New observation:** Dense blocks are created when voltage nodes are connected to nonlinear devices, all other nodes create diagonal blocks

Looking forward, this new solver provides a jumping off point

- Multi-threaded improvements to current Basker HB solver
- Use Basker HB solver on each node in parallel
- Algorithmic interpolation between Basker and block-Jacobi

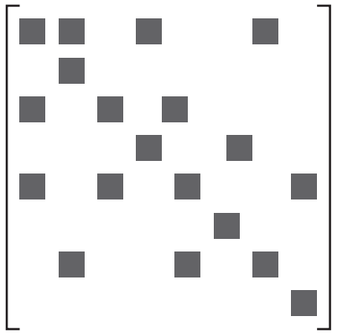
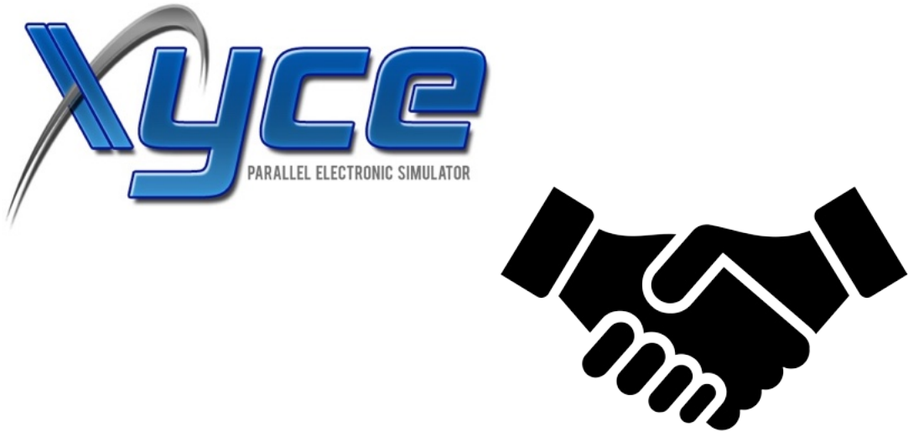


Figure 1: Sparsity structure of HB Jacobian

[4] “A robust and efficient harmonic balance (HB) using direct solution of HB Jacobian,” Mehrotra, Amit and Somani, Abhishek, DAC 2009.



Thanks to the Xyce and Trilinos teams!

Collaborators: Eric Keiter, Ting Mei, Siva Rajamanickam, Ichitaro Yamazaki, Nathan Ellingwood, David Day, Clark Dohrmann, ...