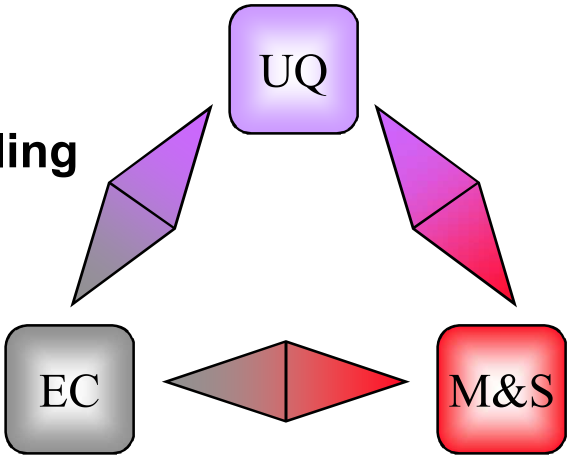
SAND2010-3341P

Qualification Alternatives to the Sandia Pulsed Reactor (QASPR)

Eric R. Keiter

Electrical and Microsystems Modeling

Albuquerque, NM



CIS External Panel Review

May 26-28, 2010

QASPR Background*

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*Covered in review talks the past two years

QASPR Context*

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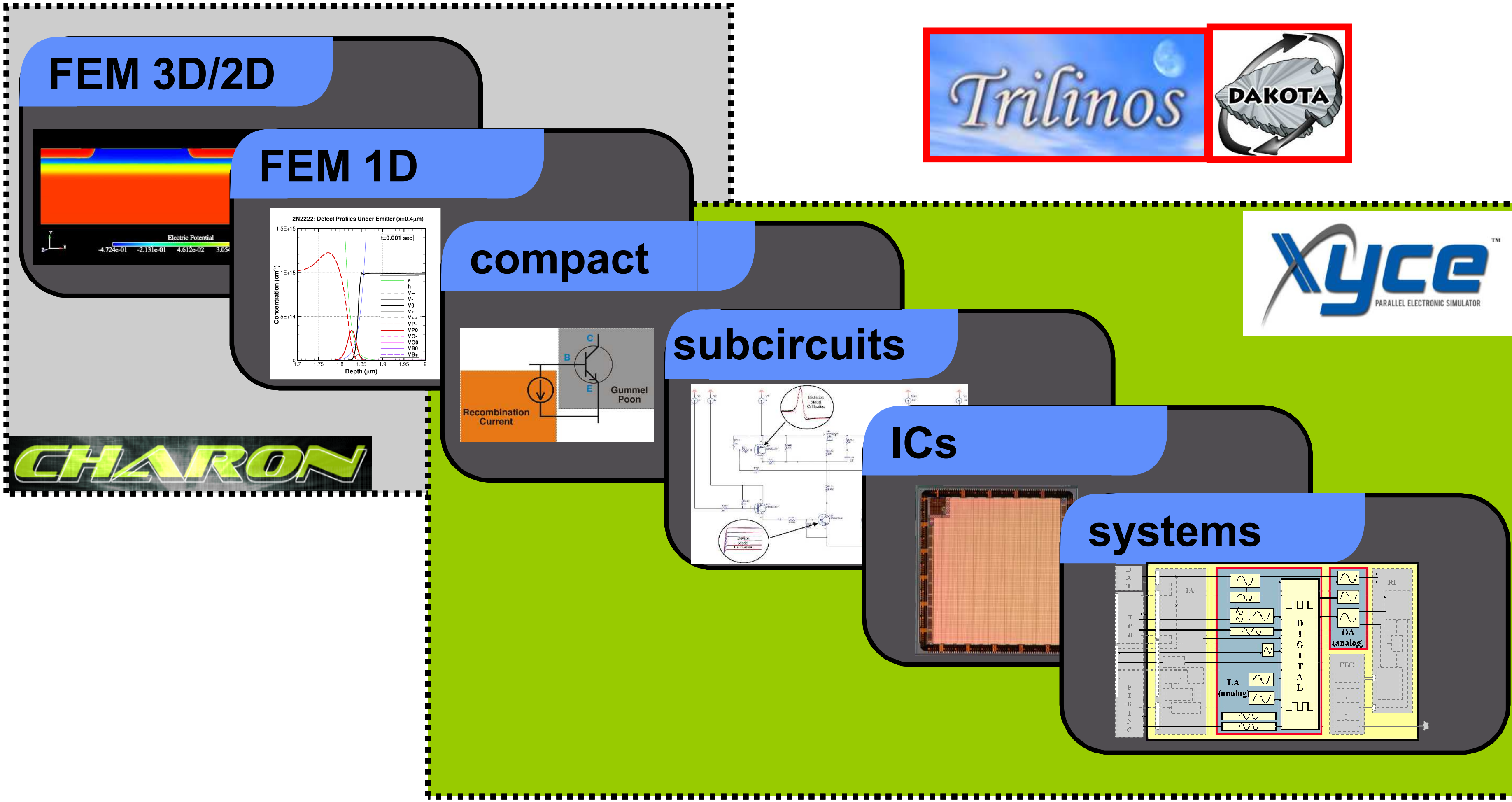
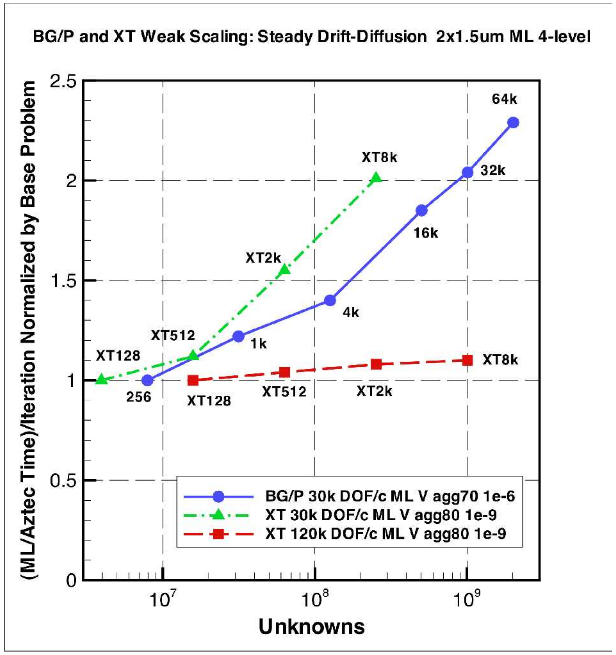
*Covered in review talks the past two years

CIS Impact:
Multi-Fidelity Modeling in RAMSES Tool Suite



CHARON Device Simulator*

- Detailed damage physics produce an order of magnitude larger problem. >30x problem size increase.
- Trilinos solvers critical to success
- Recent scaling study:
    - 2 Billion DOF
    - 65536 Cores on IBM Blue Gene/P



*Covered in review talks the past two years

Drift-Diffusion Defect Equations

$$\nabla \cdot \epsilon \nabla \psi + q(p - n + C) + \sum_{i=1}^{N} q_{Y_i} Y_i = 0 \qquad \mathbf{E} = -\nabla \psi$$

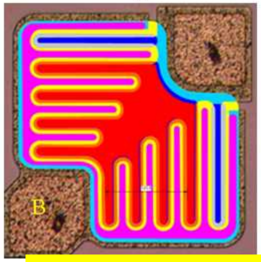
$$\nabla \cdot \mathbf{J}_n = \frac{\partial n}{\partial t} + R \qquad \mathbf{J}_n = \mu_n n \mathbf{E} + D_n \nabla n$$

$$-\nabla \cdot \mathbf{J}_p = \frac{\partial p}{\partial t} + R \qquad \mathbf{J}_p = \mu_p p \mathbf{E} - D_p \nabla p$$

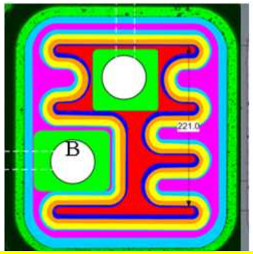
$$-\nabla \cdot J_{Y_i} - q_{Y_i} R_{Y_i} = q_{Y_i} \frac{\partial Y_i}{\partial t}$$

N>30 for Si

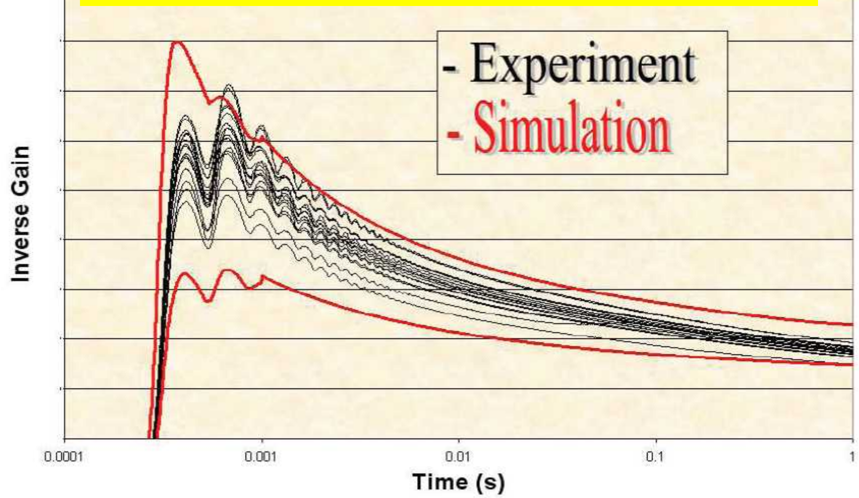
Model Development



Blind Prediction



Device Prototype Milestone, 2008*



Xyce Circuit Simulator

- **Massively parallel**
  - **Circuit-specific preconditioning**
  - **Homotopy**
  - **Reduced order modeling**
- **Radiation effects models:**
  - **x/γ–ray (ionization)**
  - **Transient N^0 (displacement damage)**
- **Impact: W76-1 AFS Qualification, QASPR, W88 LEP.**

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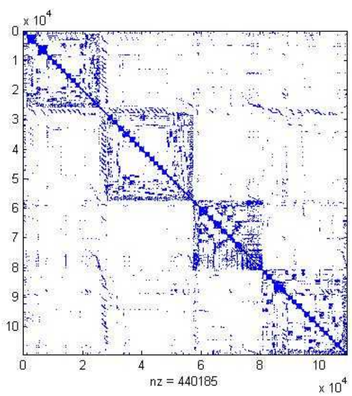
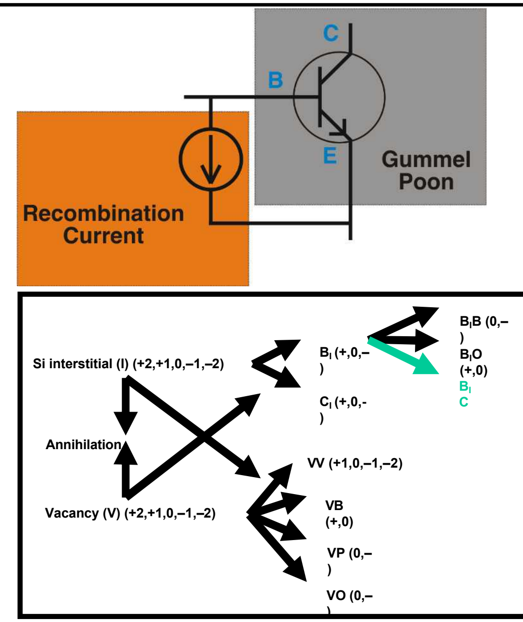
BTF+Hypergraph**



Method	Residual	Solver Time(sec)
OLD	3.4e-1	302.6
NEW	3.5e-10	0.139

100K Transistor IC Problem

**Thornquist, Heidi K., et. al., Proceedings International Conference on Computer-Aided Design, November 2009.



Compact Neutron Model*

*Keiter, Eric R., et. al., Proceedings Nuclear and Space Radiation Effects Conference, July 2010.

Complex Prototype Milestone: blind prediction of rad effects for Si circuit

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Complex Prototype Results

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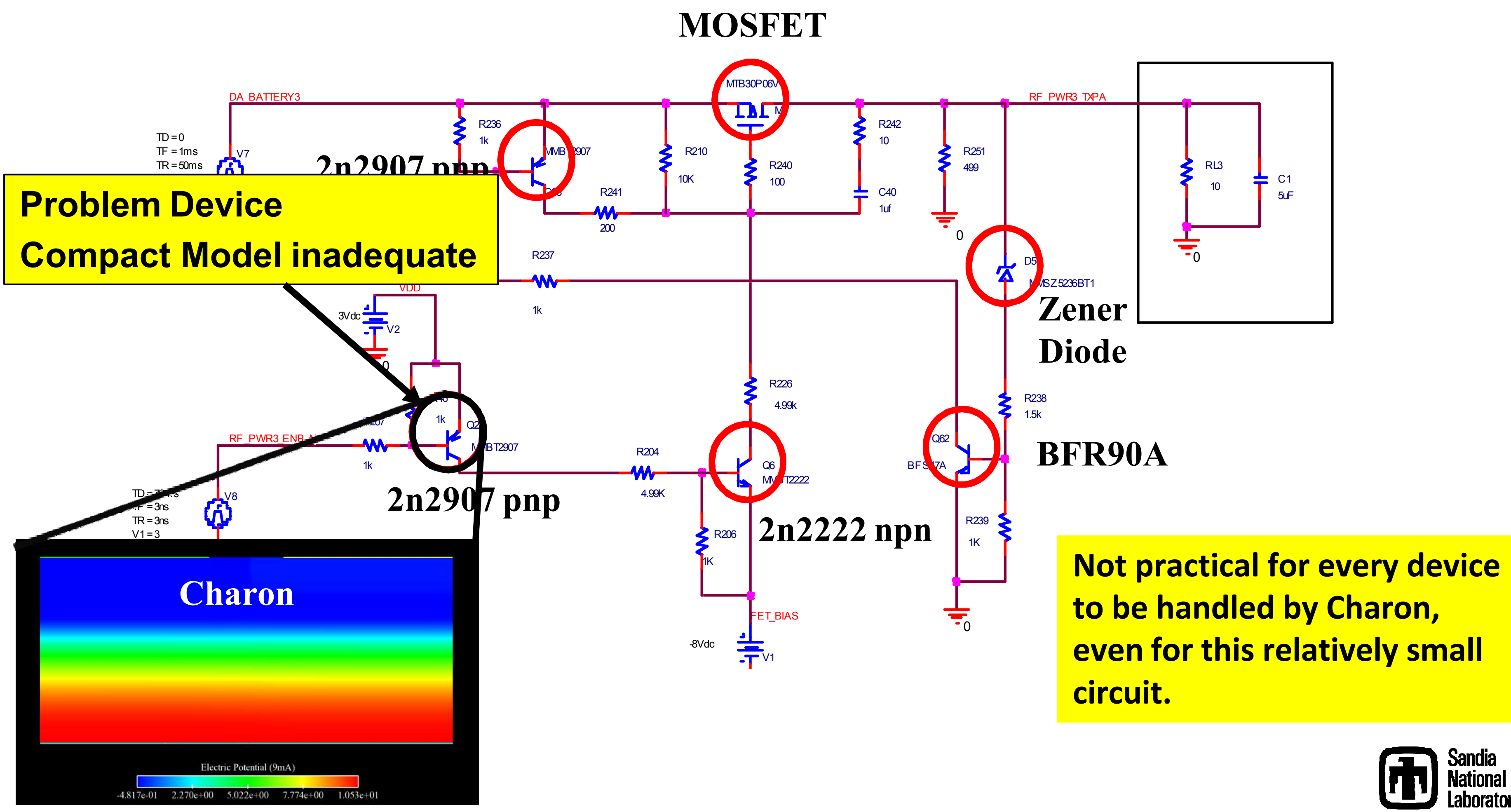
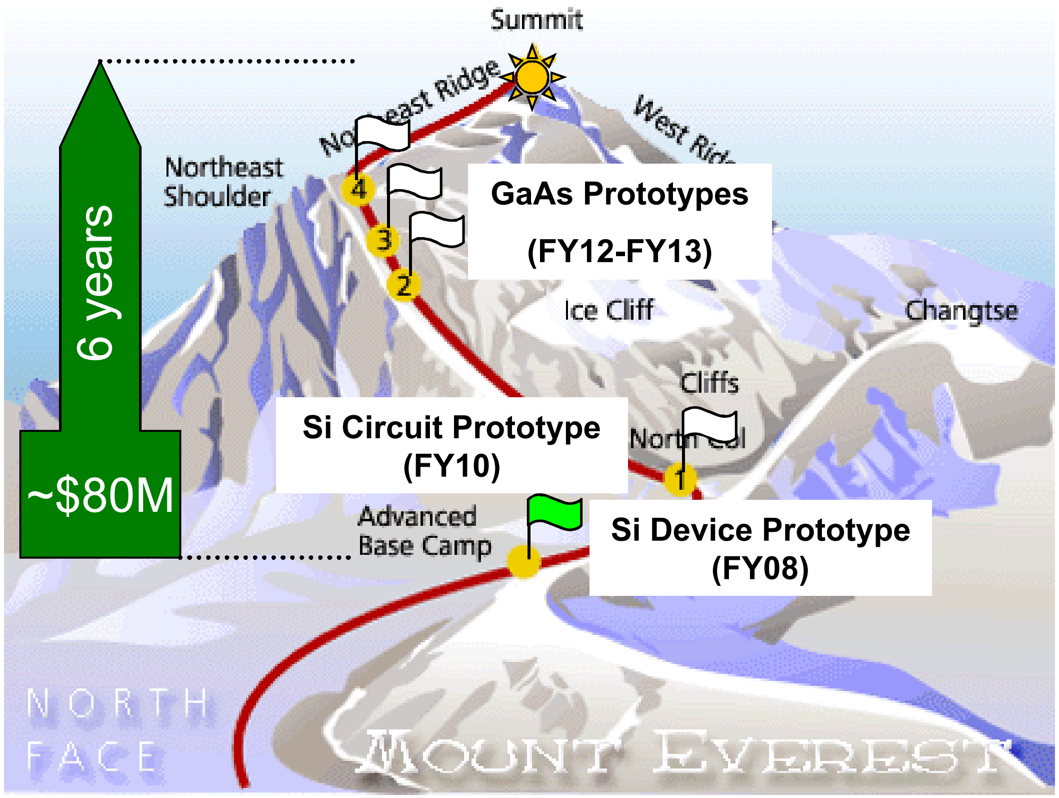
Xychron:
Charon-Xyce Coupled Simulation



Future Technical Challenges



QASPR is trailblazing a path that is transforming how we do experimental testing and qualify with confidence

- Improve computational efficiency (both Xyce/Charon)
  - Preconditioners
  - Discretization
  - Mixed-Mode coupling
  - Model Order Reduction.
- Expand device and circuit physics
  - Improve compact models
  - Clustering (multi-scale modeling)
  - New Technologies
    - Next step: III-V (GaAs)

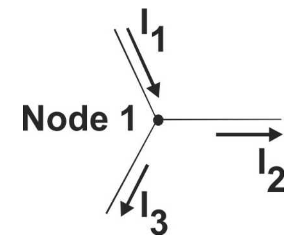
The End/Questions

Background slides: Compact Modeling of fast-burst Neutron Effects

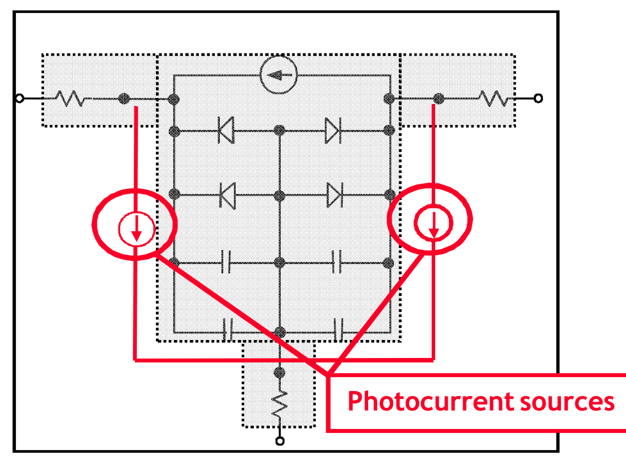
What is a "compact model"?

- Size:
  - (<10) equations per device.
  - Low fidelity
  - Computationally inexpensive
- Function:
  - provide Ohmic I-V relationships,
  - used by Xyce to enforce Kirchoff's laws (KCL equations).
- Industry-standard SPICE compact models:
  - Gummel-Poon BJT
  - BSIM3 MOSFET (over 300 parameters)
  - MEXTRAM BJT
  - VBIC (for HBTs)
- Xyce Radiation Models:
  - augment existing industry models
  - Photocurrent example, right.

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



Kirchoff's Current Law (KCL)



Photocurrent BJT

Sandia National Laboratories

History: Nomograph-Based Compact Models

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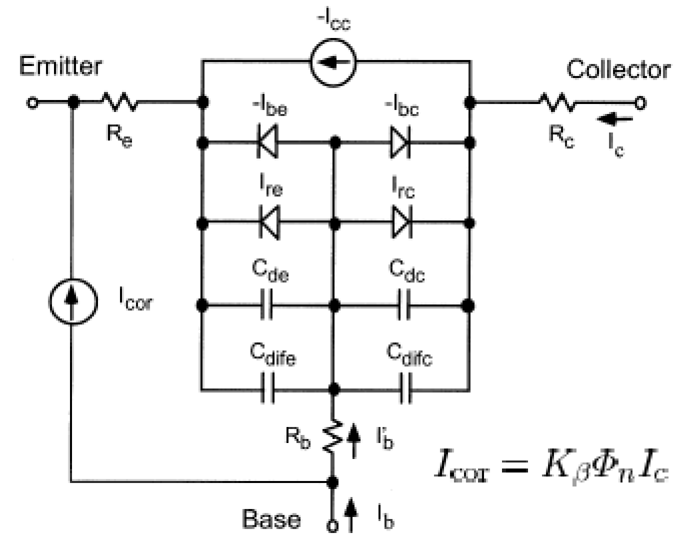
More history: Fjeldly neutron model (2003)*

- Developed for Sandia under contract.
- Forward-active only.
- Time-dependent fluence, via convolution.
- Time constant for annealing fixed by single value, τ.



$$I_{cor} = K_\beta \Phi_n I_c$$

- Numerically robust, largely because:
  - **Bias/injection dependence weak**
  - calibrated K_β param to high and low injection.
  - Rate of annealing independent of bias.

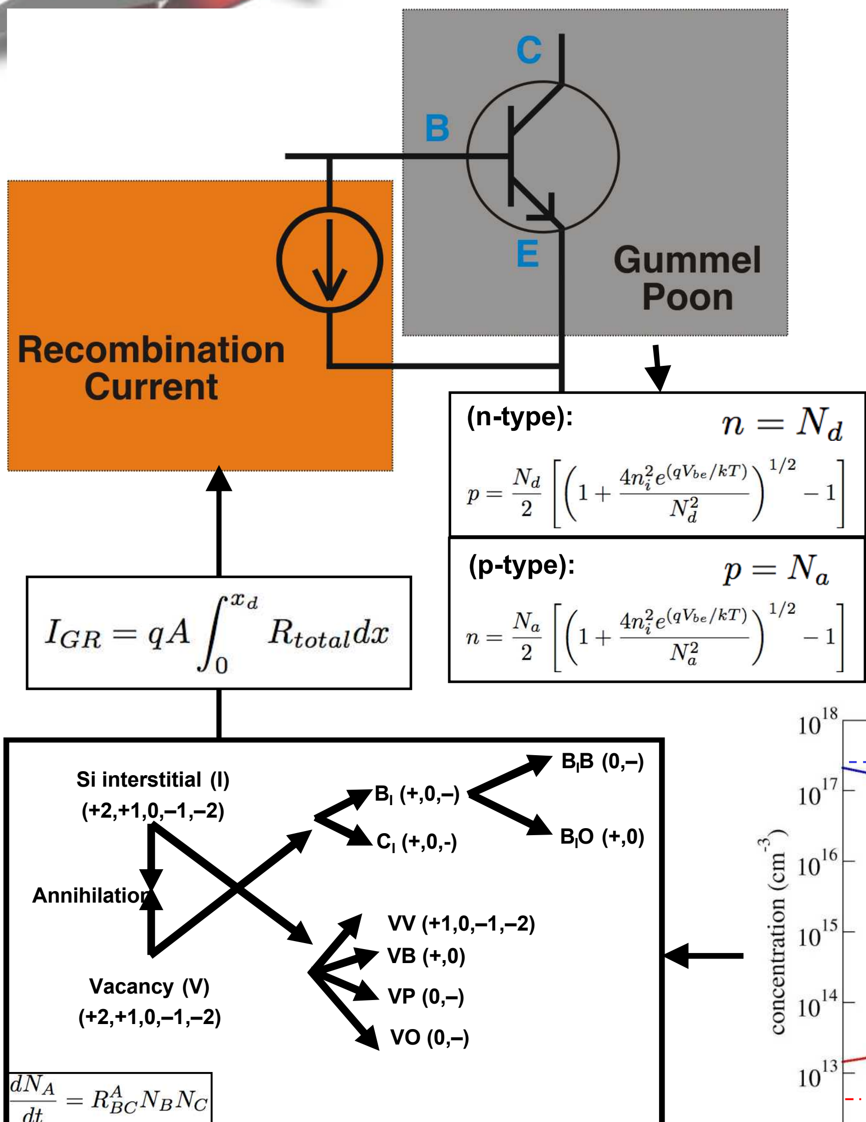
$$K_\beta = \begin{cases} a_1 I_c^{b_1}, & \text{low injection, } V_{be} < 0.4\ V \\ a_2 I_c^{b_2}, & \text{high injection, } V_{be} > 0.4\ V \end{cases}.$$

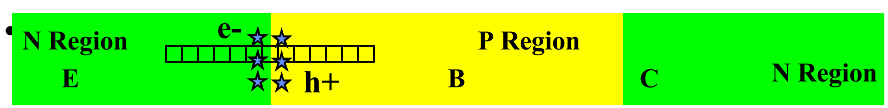
$$\Phi_n^*(t) = \int_{-\infty}^{t} F_n(t') \left[(1-\alpha_n) \exp\left(-\frac{t-t'}{\tau_a} \right) + \alpha_n \right] dt'.$$

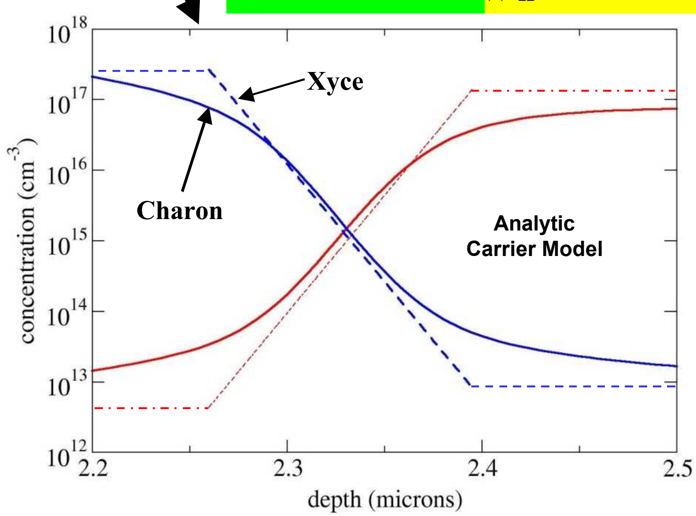
***Deng, Y, et. al., "SPICE Modeling of Neutron Displacement Damage and Annealing Effects in Bipolar Junction Transistors" IEEE Trans. Nuc. Sci., Vol. 50, No. 6, Jan. 2003, p. 1873.**

Physics-based Compact Model

- Full neutron defect reaction set.
- I_{GR} = integrated capture rates.
- Time-dependent Frenkel pair source function.
- Coupled to BJT model as parallel current source.
- Carrier density profiles approximated analytically.







Background slides: QASPR Project Scope

Sandia Pulsed Reactor III (SPR III) provided integrated testing for combined fast N^0 and Γ effects.

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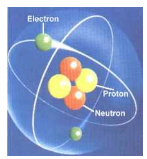
Integrated Effort Across Multiple Disciplines/Divisions: 1000, 2000, 5000, 6000, 8000, & 12000

QASPR Project Lead
Len Lorence
1341 Radiation Transport

S&T Lead
Pat Griffin
1384 Applied Nuclear Technologies



Program Manager (C7)
Mark Hedemann
1340 Radiation Effects Sciences & Applications

NNSA National Nuclear Security Administration

DSW Liaison
Bob Paulsen
2111 Technical Asst. & Deputy to 2000 VP

New Mexico Weapon Systems Engineering

- **Leadership team**

Integrated Effort Across Multiple Disciplines/Divisions: 1000, 2000, 5000, 6000, 8000, & 12000

Experimental WG Lead
Don King
1384 Applied Nuclear Technologies

- 1111 Radiation-Solid Interactions
- 1123 Semicond Material & Device Sci
- 1344 Radiation Effects Research
- 1734 Component Information & Models
- 173111 Rad Physics, Tech & Assurance

- Three working groups (WG)
- ~50 Technical Staff

Qualification & Requirements WG Lead
Joseph Castro
1437 Electrical & Microsystem Modeling

- 415 Independent Survey Assessment & Statistics
- 1411 Optimization & UQ
- 1437 Elect'l & Microsystem Modeling
- 1544 Validation & Uncertainty Quant
- 1734 Component Information & Models
- 5351 Weapon Controllers Dept.
- 6322 Infrastructure Mod & Analysis
- 6323 Ops Research & Knowledge System
- 6325 Software Engineering & Qualification Environment

Modeling & Simulation WG Lead
Sam Myers
1110 Rad, Nano & Interface Sciences

- 1111 Radiation-Solid Interactions
- 1132 CINT Science
- 1384 Applied Nuclear Technologies
- 1414 Applied Math and Applications
- 1435 Multiscale Dyn. Mat'ls. Mod.
- 1437 Elect'l & Microsystem Modeling
- 1814 Computational Mat'ls Sci & Eng
- 6325 Software Engineering and Qual Env
- 17311 Rad Physics, Tech & Assurance

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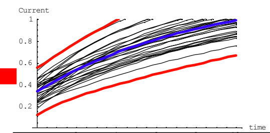
Challenge: Develop a Science-Based Engineering Methodology For Qualification

Risk Informed Decisions



Uncertainty Quantification

Qualification Evidence

UQ

EXP

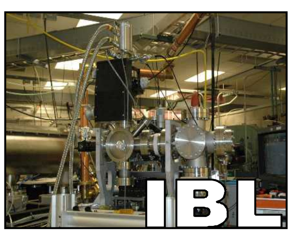
M&S

Validation

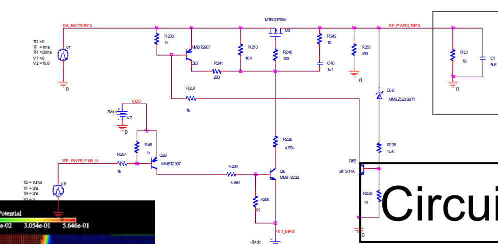
Predictive Modeling

Experimental Capabilities

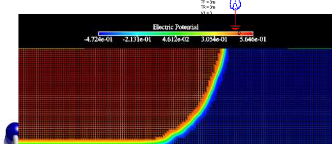
γ,n – 100 ms
long pulse



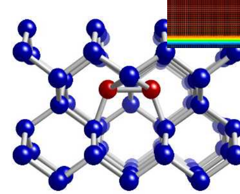
ion – 100 μs
short pulse



Circuit



Device

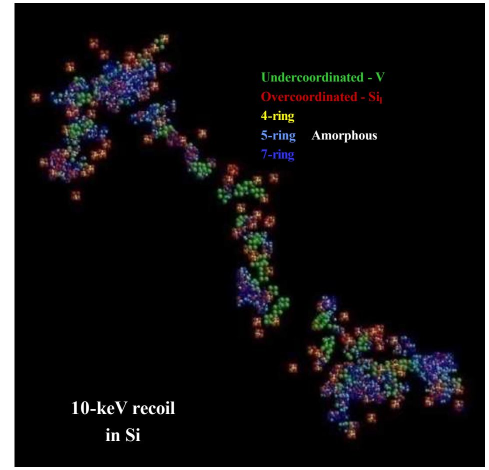


Atomistic

Developing and validating a comprehensive modeling capability.

Neutron / gamma radiation transport. → **NuGET**

Damage formation using binary collision approximation. Gives Frenkel pair maps/density and time dependent ionization. Results compared to molecular dynamics calculations → **CASCADE**



CLUSTER ← Uses Frenkel pair maps to account for defect clustering in the initial creation of defect states.

Finite element code to calculate device performance using drift-diffusion equations to model transport of carriers and defects of varying charge states. First generation uses random distribution of defect states with correction factor from CLUSTER. → **CHARON**

XYCE ← Circuit analysis code that accounts for device and circuit responses to displacement damage, photocurrent, and radiation-induced conductivity effects.

Second generation capability (in progress) will explicitly treat defect clustering within device physics code CHARON.

Background slides:
QASPR Experimental Capabilities

New experimental capabilities

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Alternative technologies may provide greater system margin than silicon BJTs.

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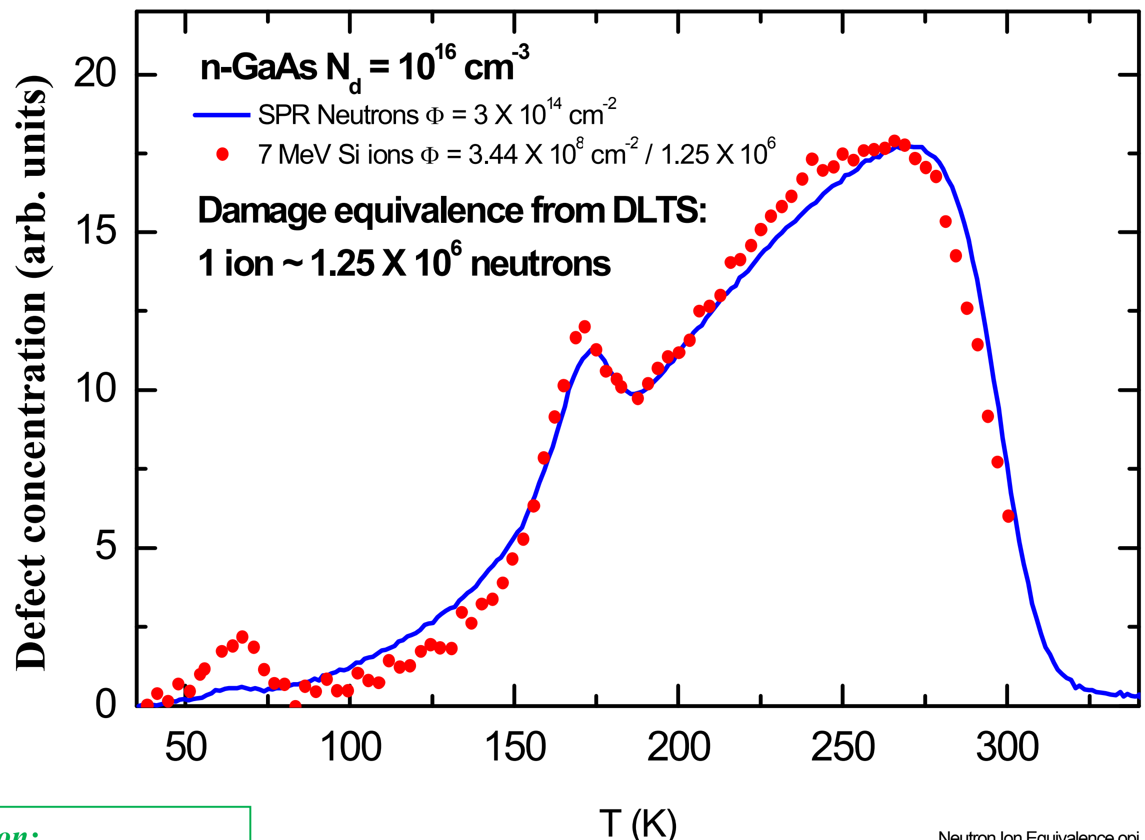
Establishing the initial damage and annealing behavior relationships between neutrons and ions is a critical element for success of the QASPR methodology for a given technology.

- We observe excellent agreement between the Deep Level Transient Spectroscopy (DLTS) spectra for SPR-III and IBL end-of-range irradiations
- Similar to our Si results, we can match DLTS spectra between neutron and ion irradiations
- These preliminary results are helping to establish initial damage relationships

This session:
Ion Irradiation of III-V (Bielejec, et. al.)

This session:
Quantifying defects in GaAs (Fleming, et. al.)

Empirical scaling used to compare SPR diode to IBL HBT



Advancement of Modeling and Simulation for III-V

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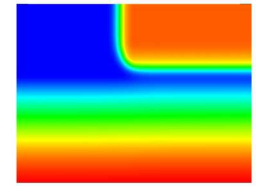
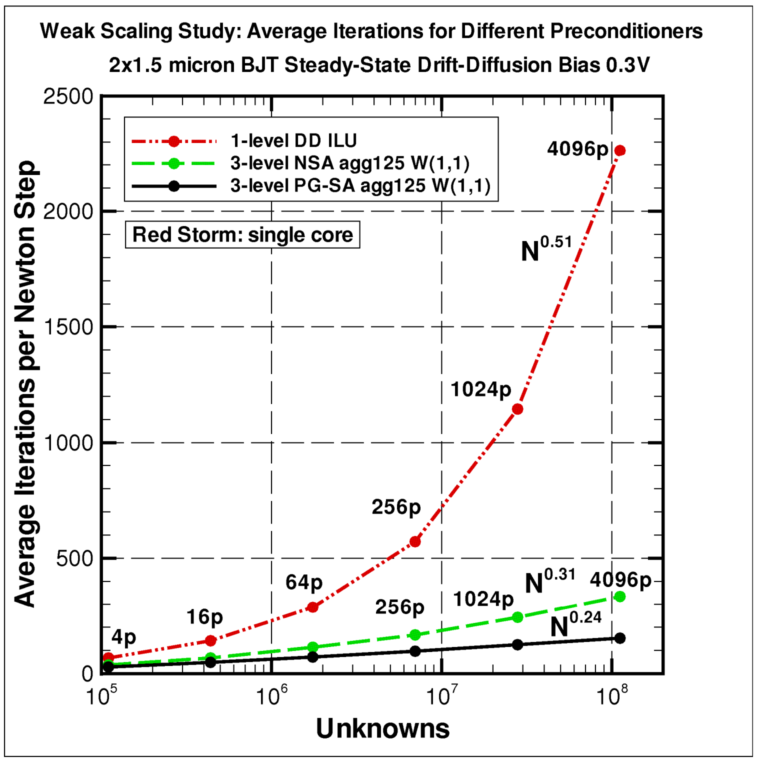
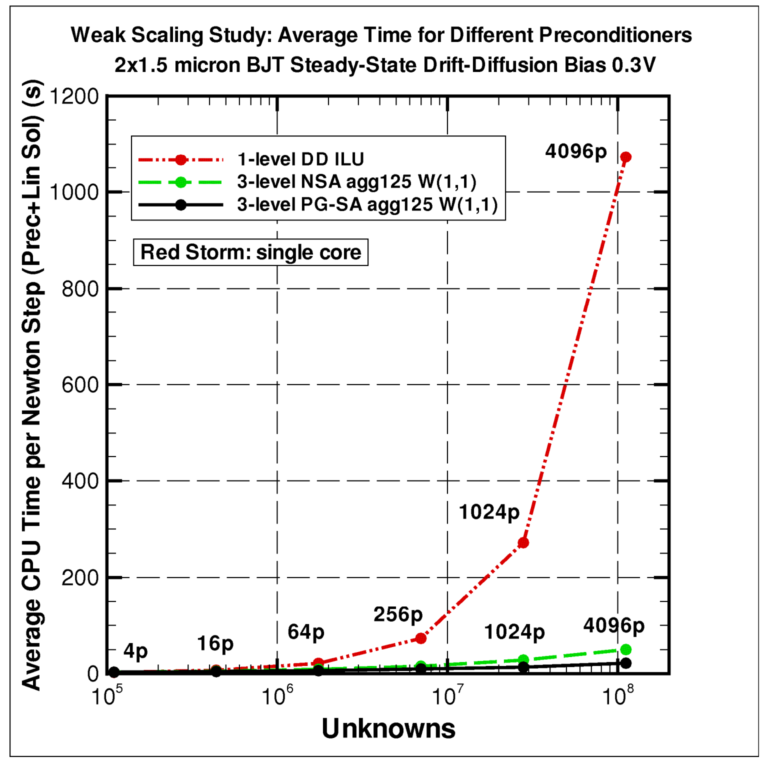
Background slides:
Charon, Xyce Parallel Scaling

Weak Scaling Study: 1-level and 3-level 2D 2x1.5 μm NPN BJT Steady-State Drift-Diffusion

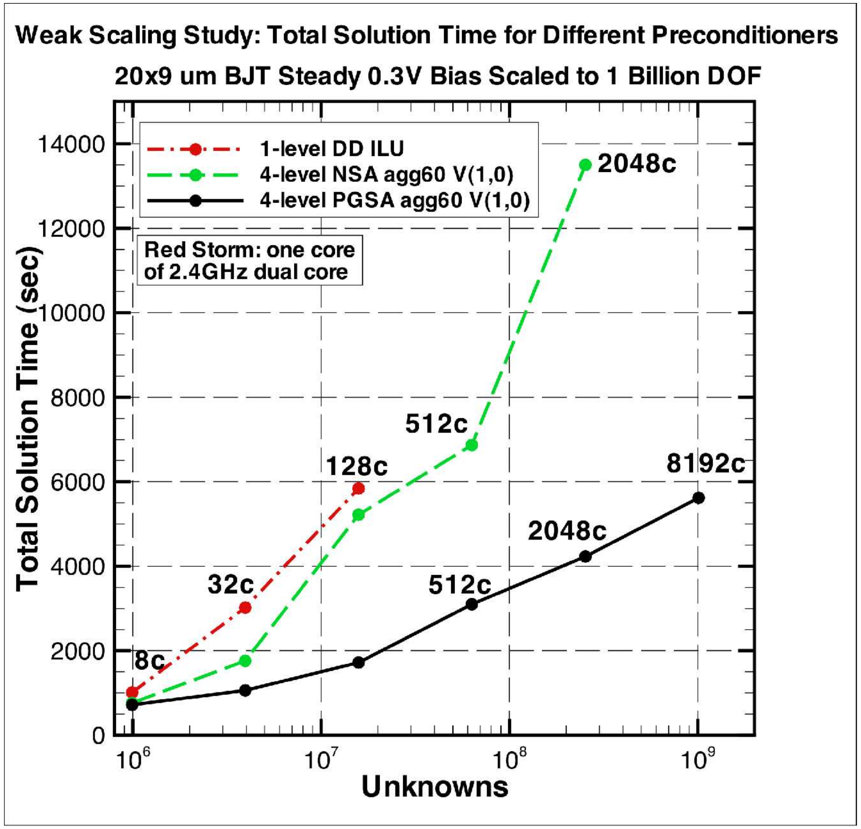
- FEM with fully implicit Newton-Krylov (GMRES) solver
- For 110M DOF run on 4096 cores of XT: PGSA 2.3 times faster than NSA; 49 times faster than 1-level







Weak scaling study: Time for 1-level and 4-level ML 20x9 μm NPN BJT Steady-State Drift-Diffusion



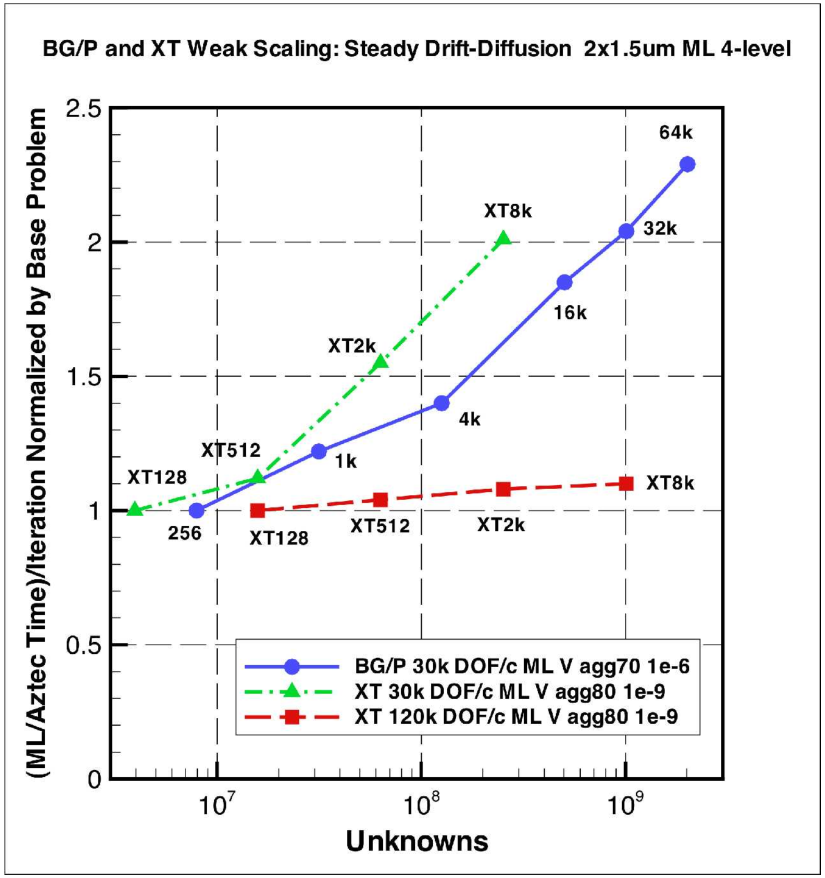
Cray XT3/4

- 4-level ML V(1,0) 60 nodes/aggregate
- Total solution time for all Newton steps
- Memory limited Krylov subspace for 1-level and ML to 600 and 550 respectively
- 1-level preconditioner did not converge for 512 core case
- Knew 4-level NSA preconditioner would not converge for 8192 core case

- PGSA preconditioner is a significant improvement over baseline NSA

DOE/NNSA

Weak Scaling to 65536 Cores on IBM Blue Gene/P



- FEM with fully implicit Newton-Krylov solver
- BJT steady-state drift-diffusion
- Problem sized increased by factor of 256 to two billion DOF on 65536 cores
- Used all four cores per BG/P node; 30k DOF/core
- TFQMR linear solver with ML PGSA 4-level
- Comparison with 30k and 120k DOF/core for Cray XT3/4: better scaling with increased work
- 2 billion DOF problem successfully run on 100k cores

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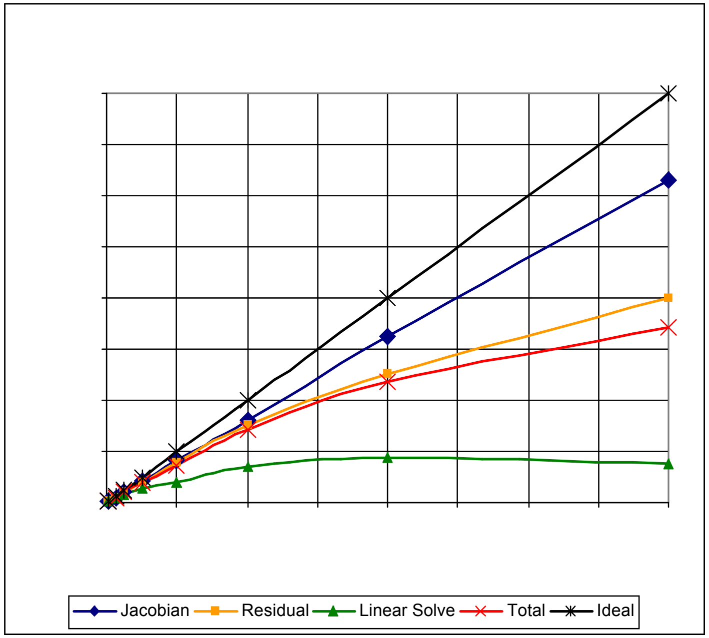
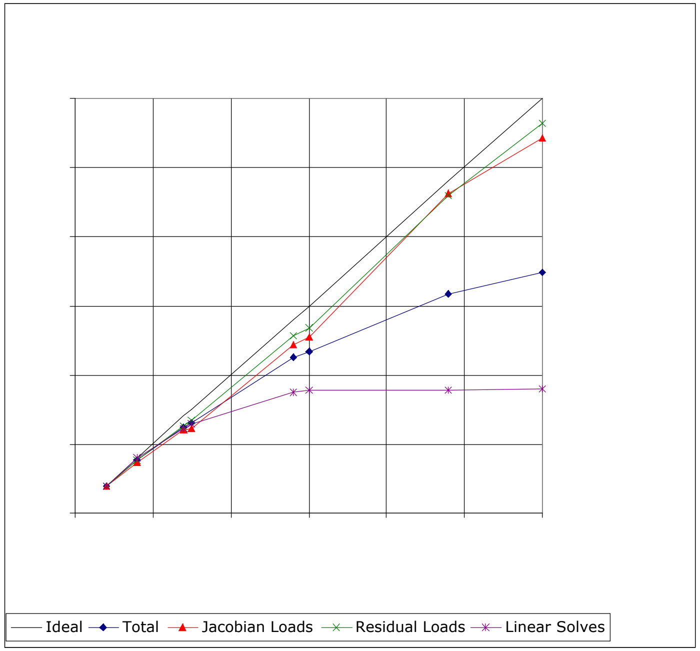
Xyce Parallel Scaling Results, circa 2003



Transmission line scaling

variable problem size



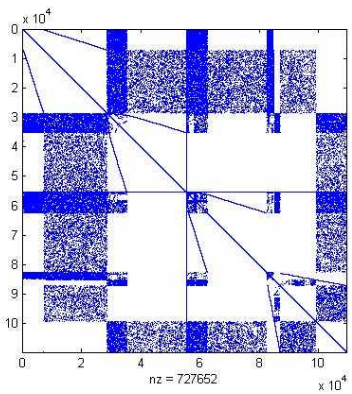
ASIC scaling

fixed problem size

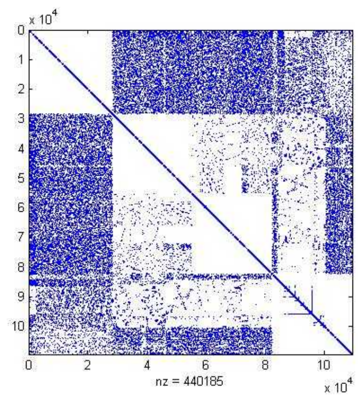
- Transmission line (max size = 14 million devices).
- ASIC scaling on the right. (much harder problem)
- For both problems, roll off occurs in the linear solve phase.

Xyce Preconditioner performance, circa 2008: 100K Transistor IC Problem

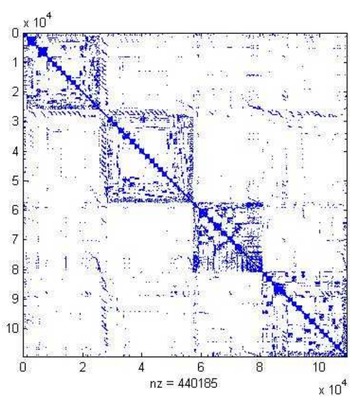
Original



ParMETIS+AMD

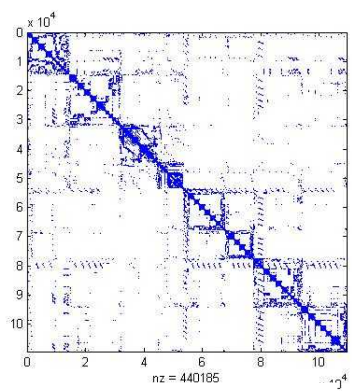


BTF+Hypergraph



4 processors

BTF+Hypergraph



8 processors

Strategy	Method	Residual	GMRES Iters	Solver Time (seconds)
1	Local AMD ILUT ParMETIS	3.425e-01	500	302.573
2	BTF KLU Hypergraph	3.473e-10	3	0.139