CEMM Meeting Agenda

8:30	Coffee Available
8:45	S. Jardin: Update on SciDAC and CERF Center News
9:00	A. Glasser -- Spectral Element Multigrid
	A. Glasser (for X. Li): PDSLin: Parallel Domain-decomp. Shur-comp. Linear Solver
9:45	N. Ferraro: New Developments with M3D-C1
10:15	break
10:30	B. Jamroz: JFNK within the semi-implicit scheme in NIMROD
11:00	C. Kim: Diagnostic development for the kinetic-MHD in NIMROD
11:30	J. King: Two-fluid tearing and saturation in pinch profiles
12:00	Lunch
1:00	H. Strauss: Disruption modeling and wall force
1:30	J. Ramos: Algorithm for the neoclassical Spitzer problem with FP collsion operator and general magnetic geometry
2:00	E. Held: Solving the DKE using 1D finite elements for pitch angle
2:30	T. Jenkins: Coupled IPS/NIMROD/GENRAY simulations
3:00	J. Breslau: Saturated n=1 mode in NSTX
3:30	break
3:45	L Sugiyama: ELMs and ELM-free instabilities
4:15	P. Zhu: MHD ballooning with RMP
4:45	J. Callen: Effect of 3D magnetic perturbations on toroidal plasmas
5:30	S. Kruger: FSP Disruption Science Driver and discussion on FSP
6:00	B. Coppi: Heavy particle mode as the signature of the I-regime.
6:30	Adjourn

CEMM Proposal was successful!

- Excellent Reviews (5 Excellent, 1 VG)
  - Technical issue: BC on disruption simulations
  - Programmatic issue: requested too much $$
- Award Letter
  - 1 of 5 FES proposals to be funded (8 were evaluated)
  - based on peer review and programmatic priorities
  - $1,050, 000 in FY11
  - Funding beyond 1st year contingent upon availability of funds, progress of the research, and programmatic needs
  - Funding for the final two years contingent upon satisfactory completion of a progress review during the third year of the project.
- John Mandrekas will provide additional guidance about what is needed in terms of revised institutional budgets next week
  - Also needs a revised scope of work for the entire CEMM project
    - . We will have a conference call to discuss this
- Recall we have promised a community-wide "kinetic-MHD closures workshop" in the 3rd year of project
  - Please start thinking about this
  - International Participants
  - Test Problems

Feedback on SciDAC

- Request from Mandrekas to present to OASCR
  - What parts of SciDAC worked well?
    - What parts did not work well?
    - Include format of annual SciDAC meeting
  - Are there areas under-represented in SciDAC

The CERF Center
Co-design for Exascale Research in Fusion
Planning Activity

BERKELEY LAB

Argonne NATIONAL LABORATORY

PPPL PRINCETON PLASMA PHYSICS LABORATORY

TECH-X

Sandia National Laboratories

Lawrence Livermore National Laboratory

GENERAL ATOMICS

PEOPLE

Principal Investigator: Alice Koniges, LBNL

Topical Leaders (Co-PI's) and Institutional Contacts:
CoDEx Design Strategy: John Shalf, LBNL
Plasma Physics: John Cary, Tech-X
Computer Science: Dan Quinlan, LLNL
Applied Mathematics: Lois Curfman McInnes, ANL
Hardware/Simulators: Curtis Janssen, SNL/CA
Fusion Code Team: Jeff Candy, General Atomics
Next Generation Fusion Codes: Steve Jardin, PPPL

Fusion Applications:

Core Transport: GYRO/NEO, Jeff Candy, Emily Belli, Aaron Collier (GA)
Collisional Edge Plasma: BOUT++, Maxim Umansky, Ron Cohen, Xueqiao Xu (LLNL)
MHD: M3D-C1, Steve Jardin, Jin Chen (PPPL); NIMROD, Carl Sovenic (Wisc), Scott Kruger (Tech-X)
Explicit PIC Modeling: GTS, Weixing Wang, Stephane Ethier (PPPL); VORPAL, Peter Messmer, David Smithe (Tech-X)

Code Integration Framework: FACETS, John Cary, Scott Kruger (Tech-X)

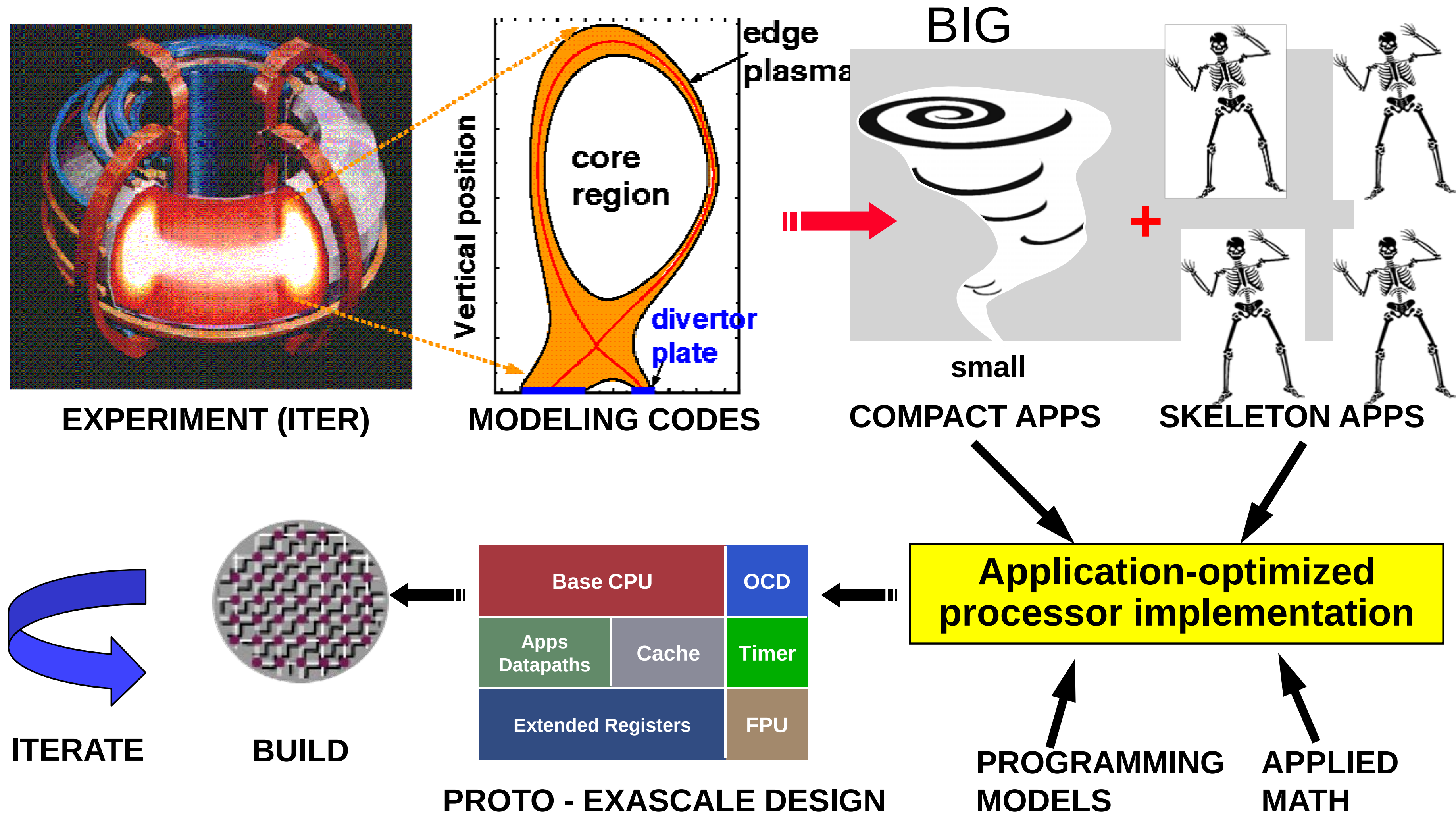
Computer Science Team:

D. Quinlan (LLNL), H. Adalsteinsson (SNL), P. Beckman (ANL), D. Camp (LBNL), H. Childs (LBNL), R. Gupta (ANL), P. Hovland (ANL), C. Janssen (SNL), C. Liao (LLNL), V. Mlaker (LLNL), B. Norris (ANL), L. Oliker (LBNL), T. Panas (LLNL), R. Preissl (LBNL), J. Shalf (LBNL), E. Strohmaier (LBNL), S. Williams (LBNL), J. Wu (LBNL)

Applied Mathematics Team:

L. C. McInnes (ANL), S. Balay (ANL), E. Constantinescu (ANL), X. Li (LBNL), B. Smith (ANL), S. Wild (ANL), C. Woodward (LLNL)

The CERF Process of Co-design



The CERF Recipe for an exascale machine

- Obtain the representative design space of applications
- Use the compact app/ skeleton app concept to connect applications with Computer Scientists and Mathematicians
- The Exascale Design Process
  - Create compact and skeleton apps
  - Analyze via tools and simulators
  - Evolve and substitute mathematical models
  - Evolve and change-out programming models
  - Create real working chips (green flash)
- Glue together using FACETS – measure with SST
- Incorporate lessons back into real codes
- Evaluate whole performance including vis and data
- Examine, evaluate, V&V
- Iterate!!

Compact Apps

- **Easy to compile, perhaps runnable on a smaller # of procs, and for a smaller amount of time**
- **Fundamentally smaller (# Lines) than full code**
- **Self-contained (data sets and input parameters)**
  - E.g., could hard code parameters
- **Strips out features that don't contribute to performance pitfalls**
- **Represents dominant features of the app**
- **Recognizes interactions between kernels**
- **Maybe more than one for each code**
- **Example GTC_simple**

Skeleton Apps

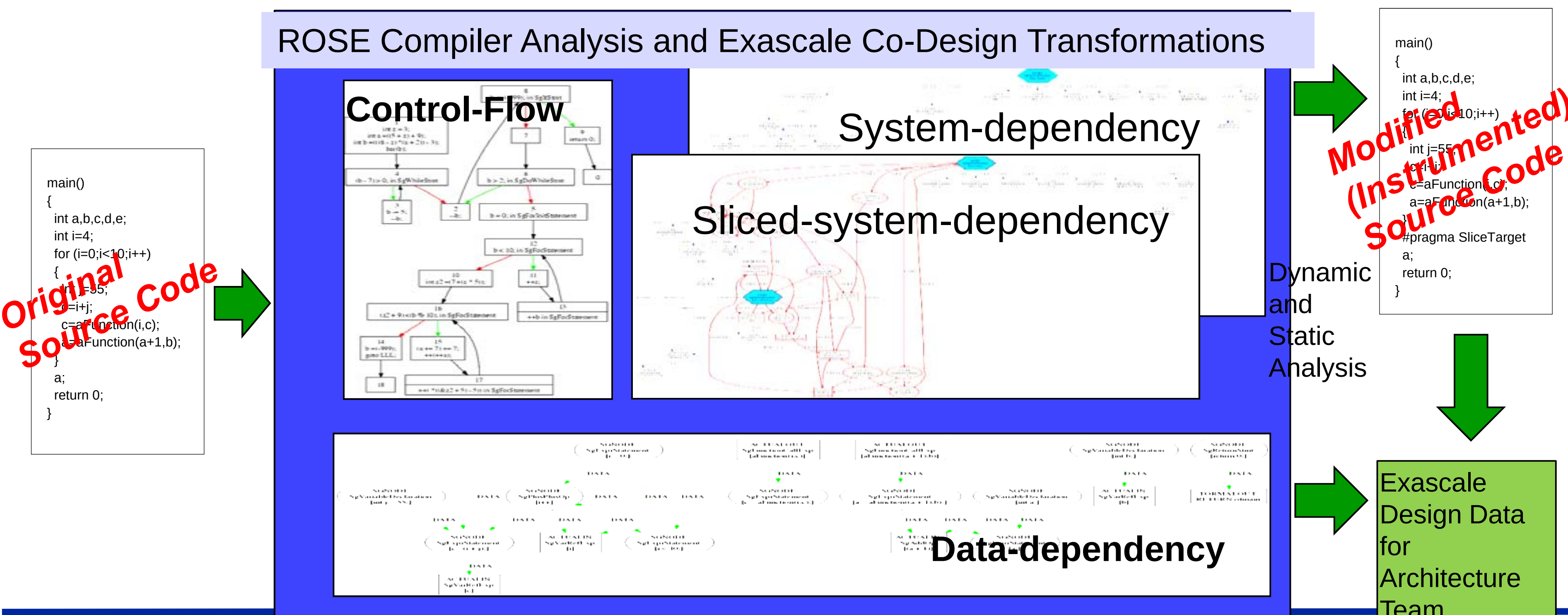
- Does not need to get correct answer
- Can be automatically generated from full application using tools, e.g., Rose
- Maybe a semi-automated path using annotations (can even be done manually)
- Focuses specific aspects of full application, e.g., flow control required for MPI communication and the MPI communication pattern
- Design to drive the simulator so we can understand performance at the extreme scale
- Skeletons feed other tools such as SST and Green Flash
- Fundamentally different from a compact app

Tools are integrated with the CoDEx methodology and performance metrics

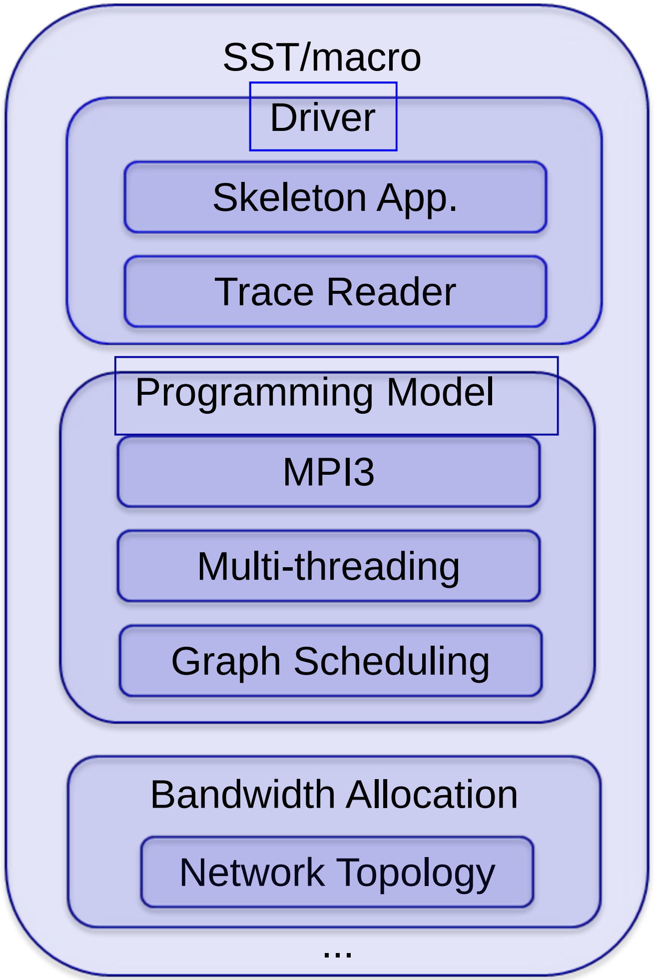
- **Rose**
- **SST**
- **RAMP/Green flash**
- **Performance tools such as IPM, Tau, OpenSpeedShop**

ROSE: Facilitating Exascale Co-Design

- **ROSE communicates subtle software design to architecture design groups**
- **Software characterization for exascale software/architecture co-design**
  - ROSE measures amount of parallelism in DOE applications
  - Classifies types of memory usage to inform hardware designers
  - Many other custom requests from exascale design teams for co-design
- **Instrumentation of apps to assess potential hardware exascale features**
- **ROSE will generate skeleton apps to drive exascale hardware simulators**

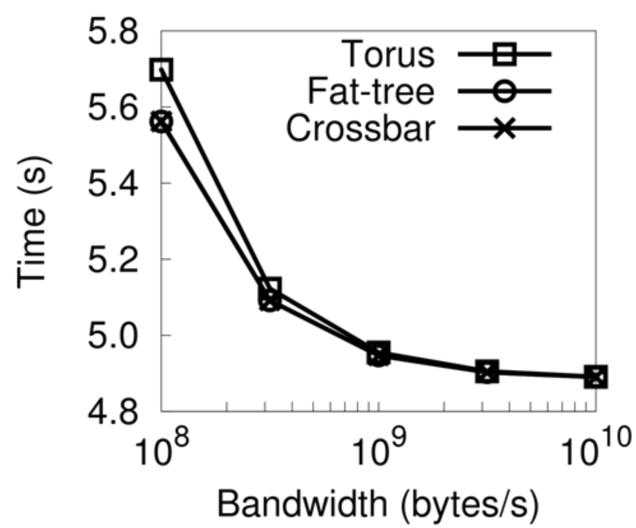


Predicting application/machine performance at full scale with the Structural Simulation Toolkit (SST)



Coarse-grained Components

Application trace collection library

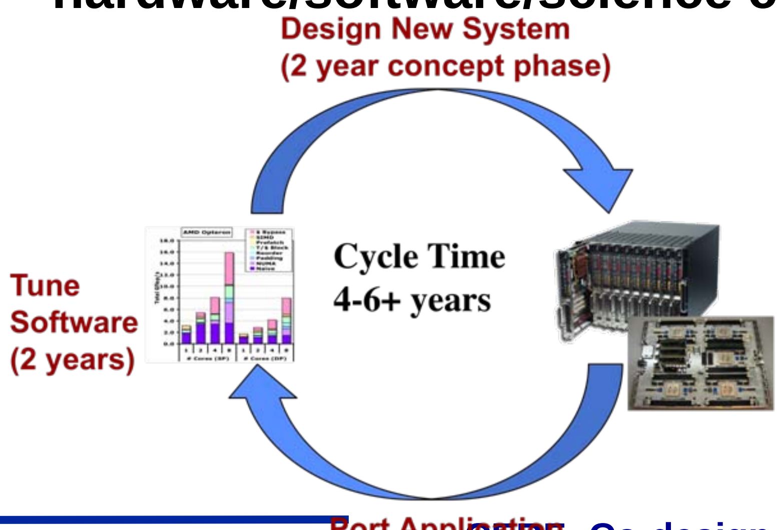


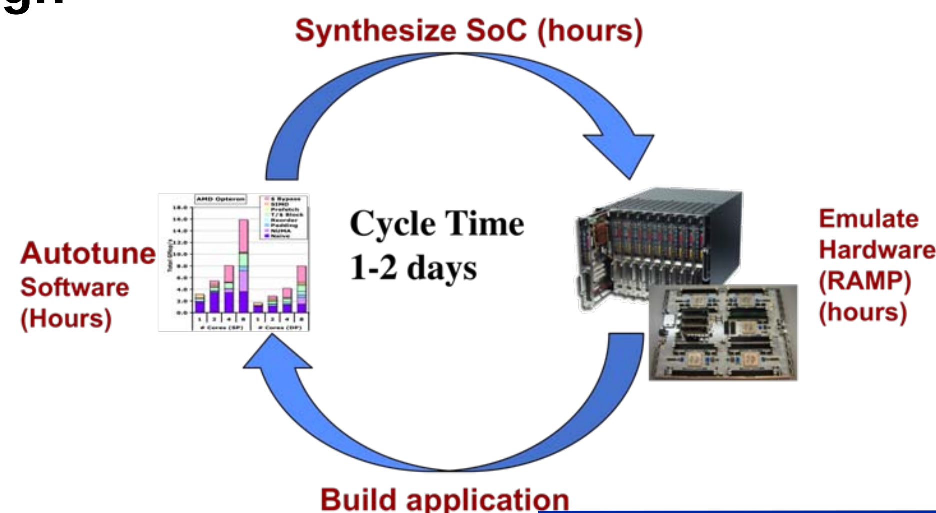
Sample performance studies using SST/macro

Have run simulations with 16,000,000 threads!

Chip-Scale Co-Design Process Emulates Feasible Design Space

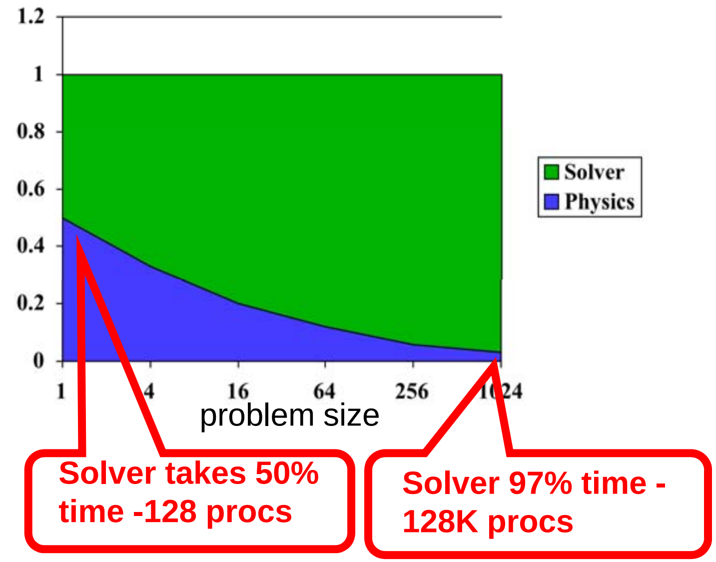
- Simulate hardware *before* it is built!
- Example: RAMP Research Accelerator for Multiple Processors
- Break slow feedback loop for system designs
- RAMP allows exploration of hardware features “in the open,” providing opportunity for vendor-specific NDA discussions in the future
- Enables tightly coupled hardware/software/science co-design





The Mathematics: Solvers, UQ, etc.

Weak scaling limit, assuming efficiency of 100% in both physics and solver phases



- **Motivating CERF Applications:**
  - Linear solvers: **M3D-C1, NIMROD, GTS, GYRO**
  - Nonlinear solvers: **BOUT++, NIMROD**, others also
  - Time integration: **BOUT++,** others also
- **Issues for Linear, Nonlinear, and Timestepping Solvers:**
  - **Efficiency:** Small numerical error/CPU cost, use appropriate integrator method for each scale/physics
  - **Scalability:** Explore operator-specific approaches to preconditioners that leverage physics knowledge; investigate novel Krylov methods that coalesce inner products, etc.
  - **Benefits:** Reduce time-to-solution; increase numerical accuracy (without sacrificing wall-time); allow finer resolution in space for a given computation time budget; benefit V&V and UQ by allowing more (optimization) iterations, more samples, or more scenarios
- **UQ Issues**
  - Tools for statistical analysis of underlying parameters and their relationship to experimental data
  - Study sensitivities to numerical errors and computational noise

Summary

- **Co-design for Fusion provides an important path to international energy solutions**
  - Not just putting off the future; a real solution
- **Integrated Co-design Center incorporates applications, computer science teams, mathematics teams, simulation elements**
- **CERF covers major code component areas for the planned FSP and includes / coordinates with FSP members**
- **Critical co-design elements presented here are dependent on funding scenarios for the co-design centers**
- **Planning activities include external review board, well-defined management plans and risk assessment, different budget scenarios**

The CERF Center

Co-design for Exascale Research in Fusion