ReveR-SES: Reversible Software Execution Systems

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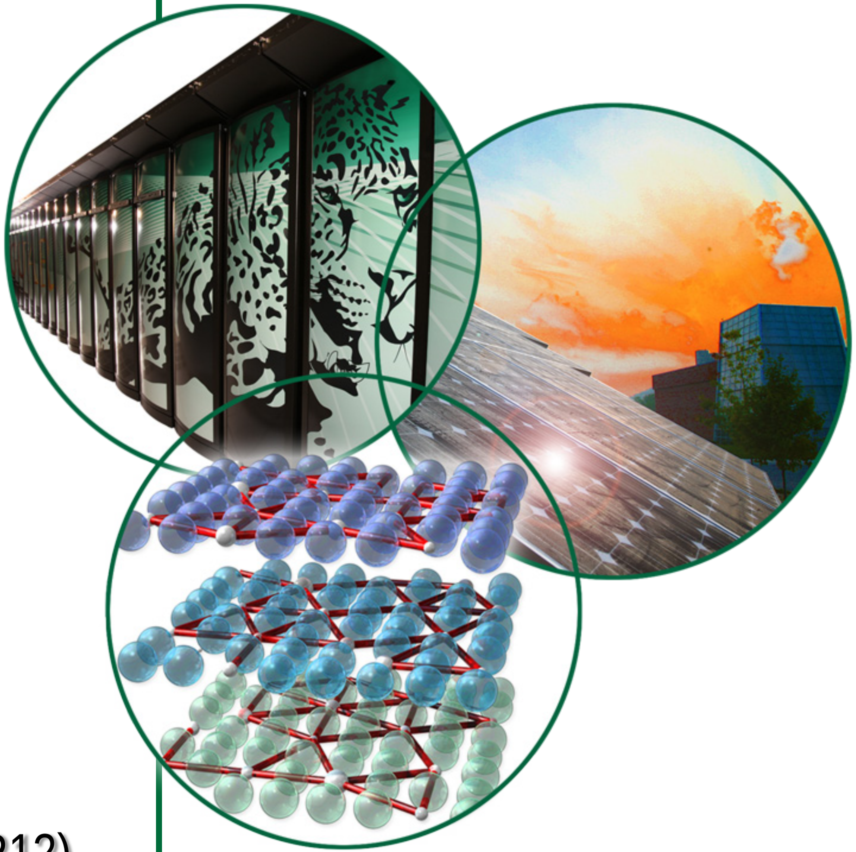

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U.S. DEPARTMENT OF ENERGY

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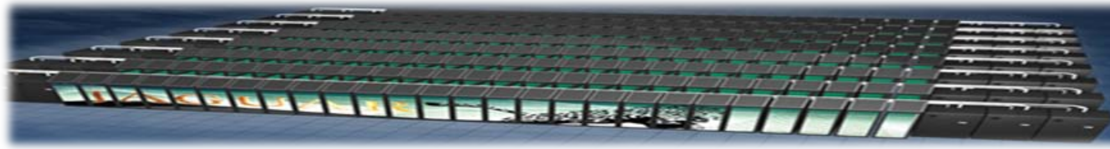
Outline

- **Introduction**
  - Problem and Solution Approach
  - Illustrations
  - Related Work
  - Research Challenges
- **Research Components**
  - Automation
  - Runtime
  - Theory
  - Experimentation
- **Summary**

Problem



- **Very large scale concurrency is burdened by inefficiency at best, and by infeasibility at worst**

  Underlying (software) challenges include synchronization, fault tolerance, and debugging

- **Need to explore paradigm alternative(s) to overcome challenges**

Simulation execution is forward-only

- Almost all current simulations, models, software are inherently forward-only

Paranoid runtime

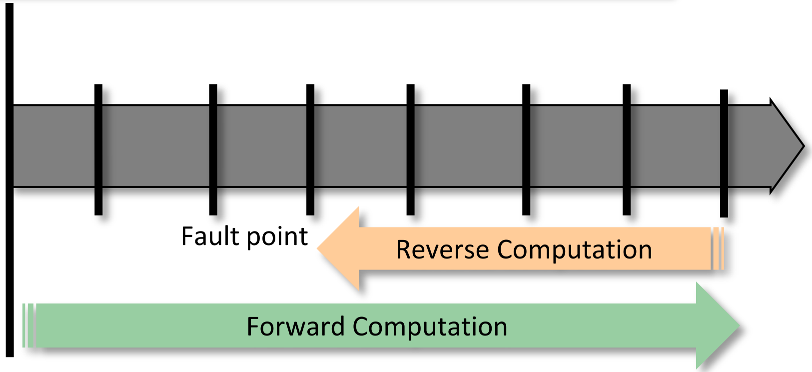
- Needs all components to be always correct

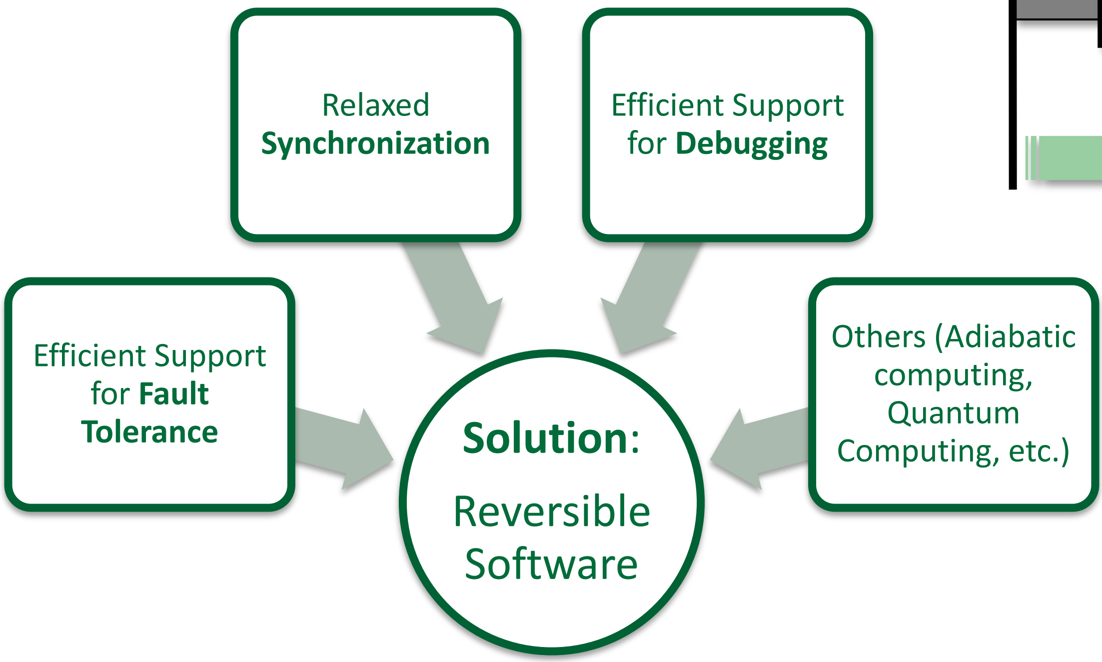
Non-scalable execution

- High synchro-nization cost
- Untenable system-wide fail-safety

Our Solution Approach

- **Relieve runtime paranoia via reversibility**
  Enable software-level reversible execution at scale
- **Perform basic research to enable efficient reversibility**
  Explore, define, refine, implement, test, experiment, study, and **advance the paradigm** of reversible execution for efficient large-scale concurrency





Simplified Illustration of Reversible Software Execution

Traditional Checkpointing	Reversible Software
Undo by saving and restoring e.g. → `{save(x);x = x+1}` ← `{restore(x)}`	• Undo by executing in reverse e.g. → `{ x = x+1 }` ← `{ x = x-1 }`
Disadvantages	Advantages
• Large state memory size	• Reduced state memory size
• Memory copying overheads slow down forward execution	• Reduced overheads; moved from forward to reverse
• Reliance on memory increases energy costs	• Reliance on computation can be more energy-efficient

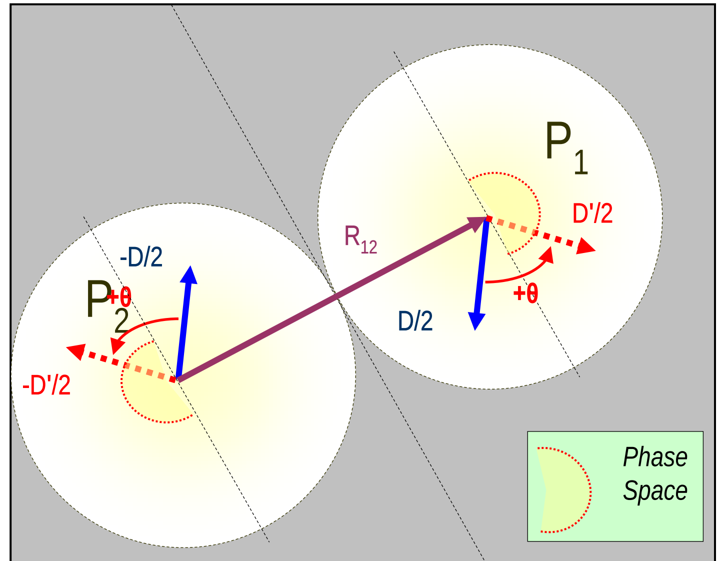
Illustration of a More Complex Reversible Model Execution

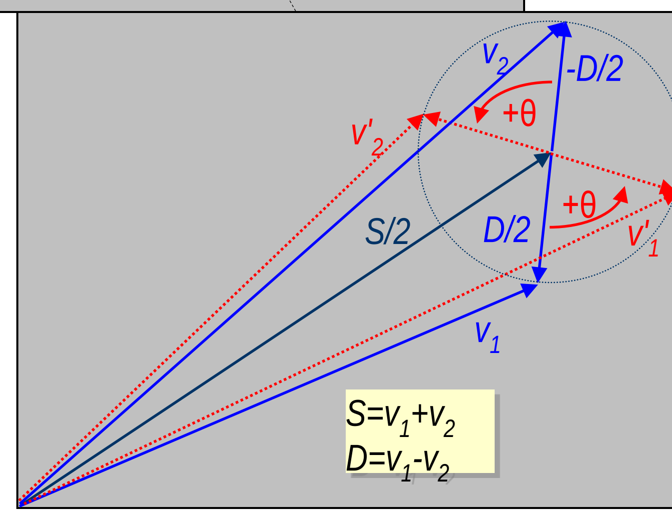
- Example: Simulate elastic collisions reversibly
  - n-particle collision in d dimensions, conserving momentum and energy
  - Incoming velocities X‘, outgoing velocities X
- Traditional, inefficient solution
  - In forward execution, checkpoint X'
  - In reverse execution, restore X‘ from checkpoint
  - Memory M proportional to n, d, and #collisions N_c

    $M=n\times d\times 8\times N_c$ bytes
- New, reversible software solution
  - Generate new reverse code
  - In forward execution, no checkpoint of X'
  - In reverse execution, invoke reversal code to recover X‘ from X
  - Memory dramatically reduced

    E.g., for n=2, 1 bit per collision
  - In fact, zero-memory can also be achieved!

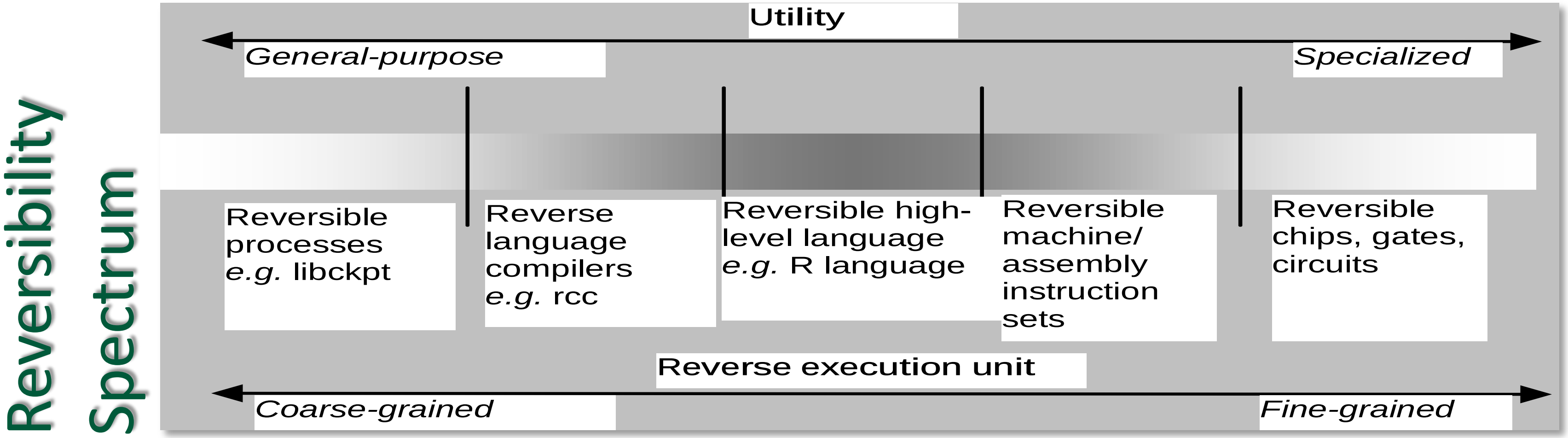
    We have now solved it for n=2, 1≤d≤ 3, and n=3, d=1





Related Work

Time warp, VLIW, Trace scheduling, Adiabatic circuits, Speculative execution, Database Transact., Undo-redo, Functional programming, Cellular automata, Thermodynamics, Quantum computing, …



	Forward-only	Reversible
Synchronous	Old paradigm of all traditional parallel computing	A sub-optimal variant, but improved scalability than forward-only
Asynchronous	Other emerging paradigms (Non-blocking collectives, new languages, programming models, etc.)	**Our proposed new paradigm of fully generalized, staggered, reversible execution by all processors**

Reversible Software: Challenge

- **Conceptually appealing at a high level, but very hard to realize in practice**
- **With very few exceptions, most existing simulations are irreversible**

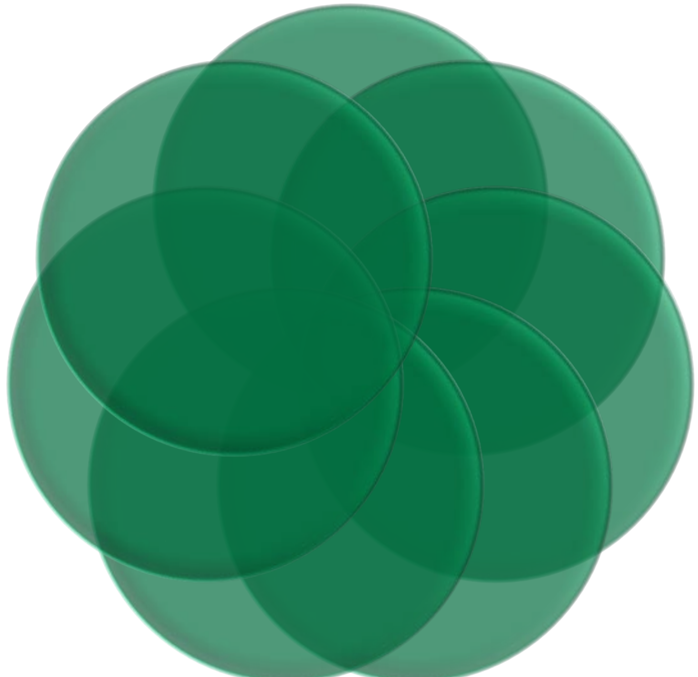
  Very complex control flows, data structures, inter-processor dependencies
- **Almost all existing approaches for undoing computation rely on *memory*, *not* true (reverse) *computation* software**
- **Need theory, methodology, frameworks, proofs-of-concept, and scaling demonstrations to advance reversible software**

Selected Research Challenges in Reversible Software

Generate efficient reversible models of physical systems

(Semi-) Automatically make existing models/code reversible (reverse compiler)

Implement, establish feasibility, and optimize reversibility at scale



Develop backward-compatible interfaces for reversibility

Develop efficient runtime engines for reversible execution at scale

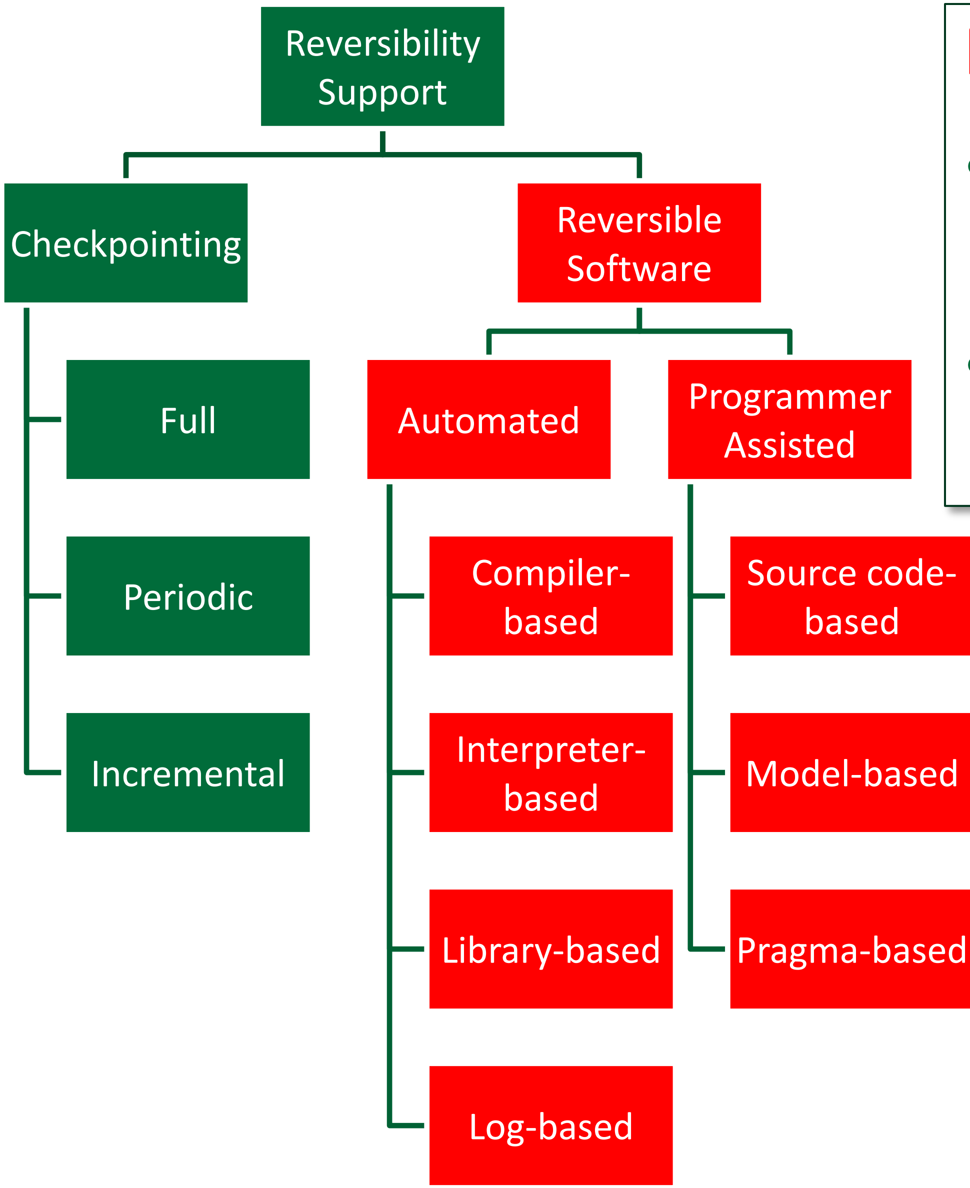
Determine trade-off between reversal, re-computation, and memory costs

Determine, and achieve, memory lower bound for efficient reversibility

Principal Research Components

Automation	Reverse compilers, reversible libraries, …
Runtime	Execution supervisor, extensions to standards, …
Theory	Memory limits, novel modeling approaches, methodologies, …
Experiments	Experimentation system, benchmarks, mini-apps, scaling, …

Our Automation Approach

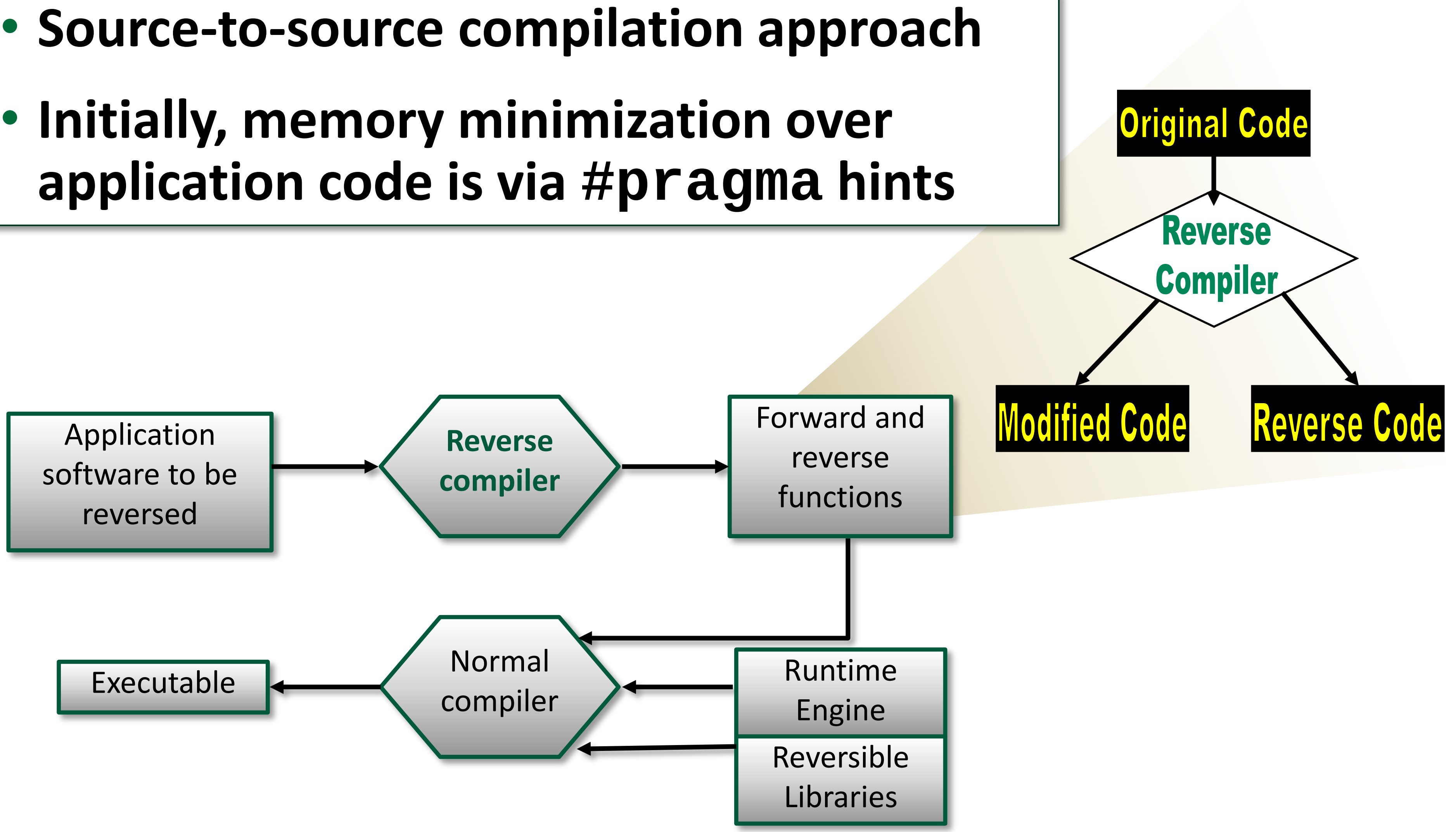


Reversible Software

- **Fundamentally distinct from checkpointing**
- **Theoretically, a strict superset of checkpointing**

Automation (cont.) – Compiler-based

- **Source-to-source compilation approach**
- **Initially, memory minimization over application code is via `#pragma` hints**



Automation (cont.) – Basic Reversal Methodology for Source-to-Source

- Simple generation rules as starting points for reverse source generation, and *upper-bounds* on bit requirements for various statement types
- Much optimization necessary at a higher-level, beyond these rules

Type	Description	Application Code			Bit Requirements		
		Original	Translated	Reverse	Self	Child	Total
T0	simple choice	if() s1	if() {s1; b=1;}	if(b==1){inv(s1);}	1	x1,	1+
		else s2	else {s2; b=0;}	else{inv(s2);}		x2	max(x1,x2)
T1	compound choice	if () s1;	if() {s1; b=1;}	if(b==1) {inv(s1);}	lg(n)	x1,	lg(n) +
	(n-way)	elseif() s2;	elseif() {s2; b=2;}	elseif(b==2) {inv(s2);}		x2,	max(x1….xn)
		elseif() s3;	elseif() {s3; b=3;}	elseif(b==3) {inv(s3);}		….,	
		else() sn;	else {sn; b=n;}	else {inv(sn);}		xn	
T2	fixed iterations (n)	for(n)s;	for(n) s;	for(n) inv(s);	0	x	n*x
T3	variable iterations	while() s;	b=0;	for(b) inv(s);	lg(n)	x	lg(n) +n*x
	(maximum n)		while() {s; b++;}				
T4	function call	foo();	foo();	inv(foo)();	0	x	x
T5	constructive	v@ = w;	v@ = w;	v = @w;	0	0	0
	assignment						
T6	k-byte destructive	v = w;	{b =v; v = w;}	v = b;	8k	0	8k
	assignment						
T7	sequence	s1;	s1;	inv(sn);	0	x1+	x1+…+xn
		s2;	s2;	inv(s2);		….+	
		sn;	sn;	inv(s1);		xn	
T8	Nesting of T0-T7	Recursively apply the above			Recursively apply the above		

Automation (cont.) – Model-based Reversal Example

Diffusion Equation

$$\frac{\partial F}{\partial t} = k\frac{\partial^2 F}{\partial x^2} + \alpha$$

Forward

$$a_i^{j+1} = k\Delta t\frac{(a_{i+1}^j + a_{i-1}^j) + (2 - \frac{\Delta x^2}{k\Delta t})a_i^j}{(\Delta x^2)} + \alpha\Delta t$$

Reverse

$$a_i^j = \frac{k\Delta t(a_{i+1}^j + a_{i-1}^j) - (\Delta x^2)a_i^{j+1} + \alpha(\Delta x^2)\Delta t}{(\Delta x^2) - 2k\Delta t}$$

Discretization

$$\frac{a_i^{j+1} - a_i^j}{\Delta t} = k\frac{a_{i+1}^j - 2a_i^j + a_{i-1}^j}{(\Delta x)^2} + \alpha$$

Reversible Execution

- Space discretized into cells
- Each cell *i* at time increment *j* computes a_i^j
- Can go forward & reverse in time
  - Forward code computes a_i^{j+1}
  - Reverse code recovers a_i^j
- Note that $a_{i+1}^{j+1} = a_{i+1}^j$ due to discretization across cells

Automation (cont.) – Linear Codes

Compute n^th^ and n+1^th^ Fibonacci number: f(n)=f(n-1)+f(n-2)

int a = 0, b = 1

Forward

for *i* from *2* to n:
    Invoke f()

```
f()
{
        int c = a
        a = b
        b = b + c
}
```

Reverse

Reverse

for *i* from *n* to 2:
    Invoke $f^{-1}()$

```
f-1()
{
        int c = a
        a = -a + b
        b = c
}
```

i		2	3	4	5	6
a	0	1	1	2	3	5
b	1	1	2	3	5	8
c		0	1	1	2	3

$f^{-1}(f(a,b)) = (a,b)$

$f^{-1}(f^{-1}(f(f(a,b)))) = (a,b)$ ...

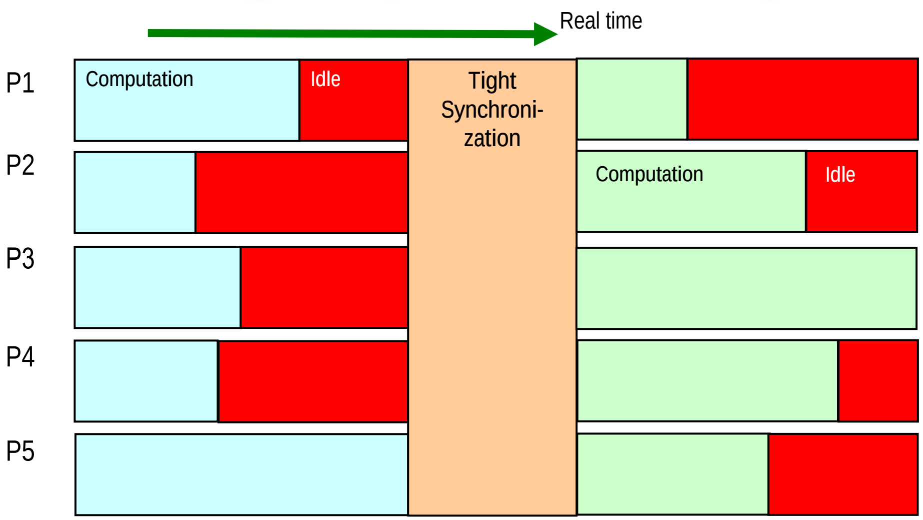
In general, can reverse linear codes, by using single static assignment (SSA), inversion and reduction. *Examples*: Swap, Circular Shift

Automation (cont.) – Libraries

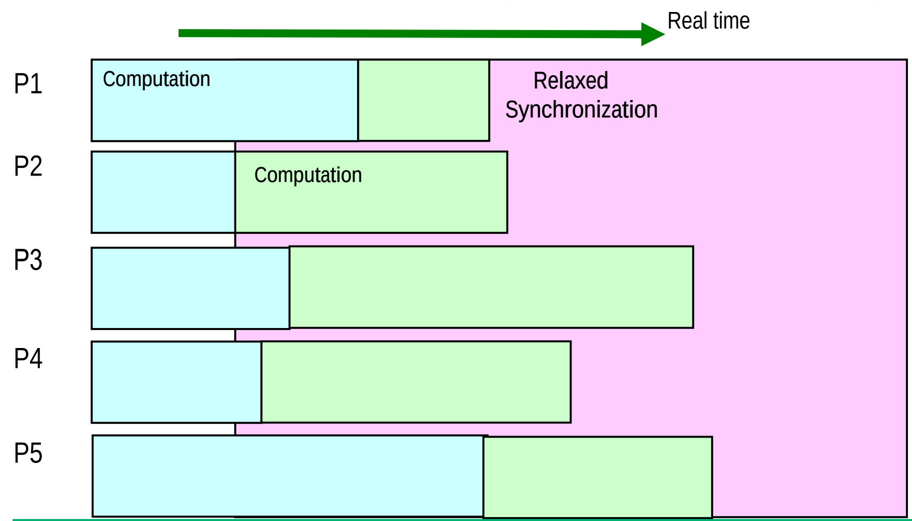
- **Reversible versions of commonly-used libraries**
- **Example 1: Random number generation**
  - Reversible random number generator RRNG (to be released soon) in C, Java, and FORTRAN
  - Large period, multiple independent streams
- **Example 2: Reversible data structures**
  - We are developing container data types with forward and reverse modes
- **Example 3: Reversible linear algebra**
  - We are developing a first cut at Rever-BLAS (Reversible Basic Linear Algebra Services)

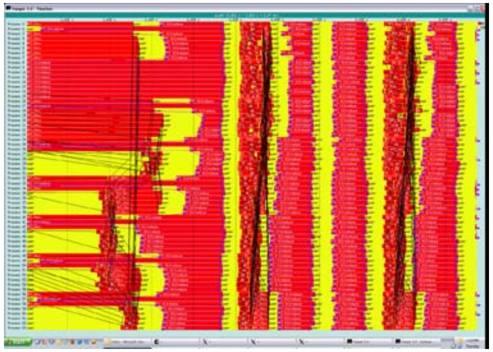
Reversible Runtime: Relaxation of Synchronization

Tight (traditional)



Relaxed (reversible)





E.g., Vampir Trace of
Parallel Ocean Program (POP)

Local and Global Causality

- Causal errors detected and corrected at runtime
- Intra-processor reversal with anti-computation
- Inter-processor reversal with anti-messages
- Runtime performs intermediate message buffering and flow control

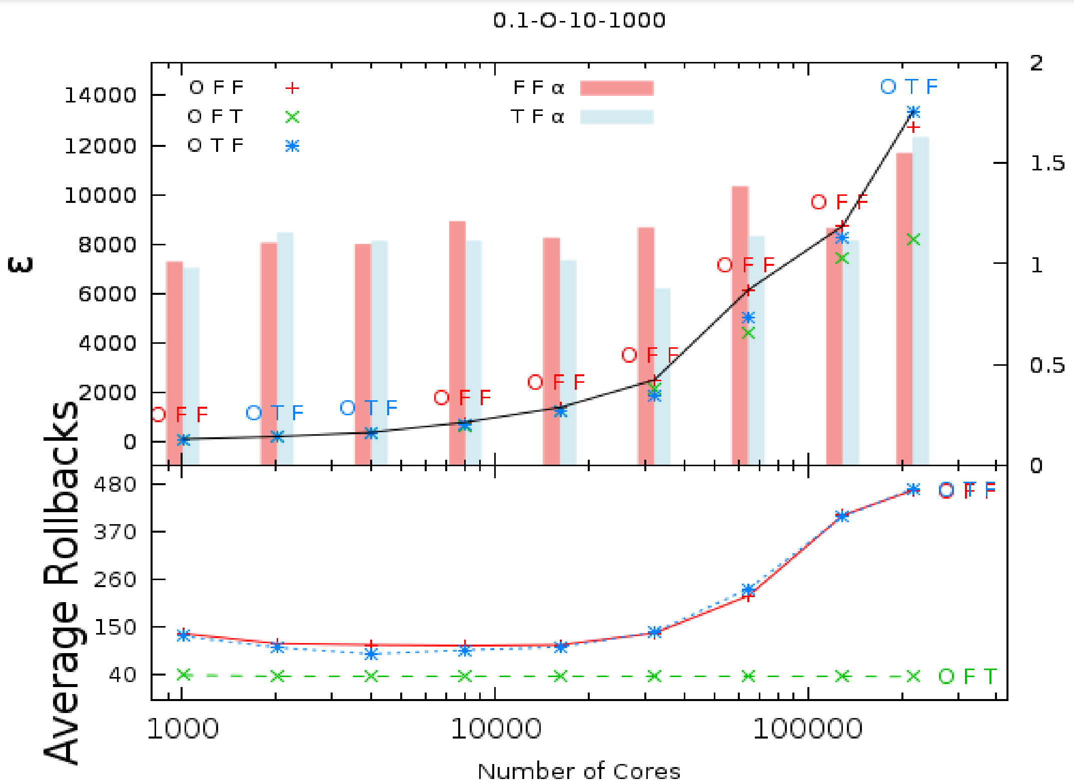
Reversible Runtime (cont.) – Feasibility

- **Relatively fine-grained GUPS-like model**
  - discrete event model, hand-coded reverse code, model size increased with no. of cores (weak scaling), randomized processor neighborhood of ±100
- **Reversible asynchronous execution achieved with high efficiency**

Executed on up to 216K cores of Jaguar (Cray XT5)

ε = millions of events/second

α = factor of improvement over synchronous execution



Reversible Runtime (cont.)

- **Reversible execution of a reaction-diffusion process model**
- **High efficiency achieved at scale, with low-level Portals communication layer; over 2× faster than synchronous mode**

Reaction:

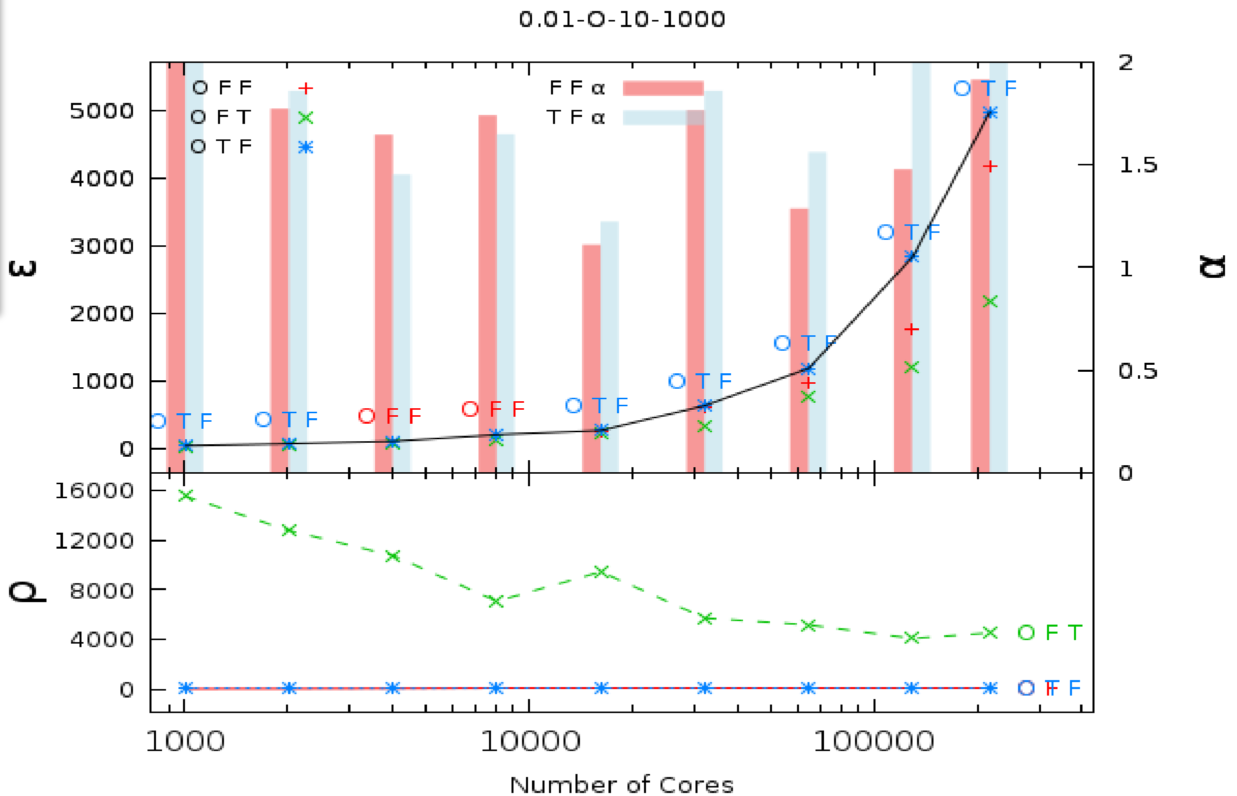
$$p_i = 1 - e^{t \sum_{r \in R} N_r \ln(1 - r s_i \rho)}$$

Diffusion:

Exponentially distributed dwell times, travel times

Executed on up to 216K cores of Jaguar (Cray XT5)

ε = millions of events/second
ρ = average number of rollbacks per core
α = factor of improvement over synchronous mode



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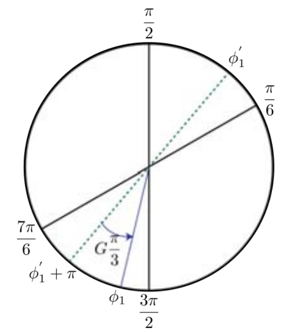
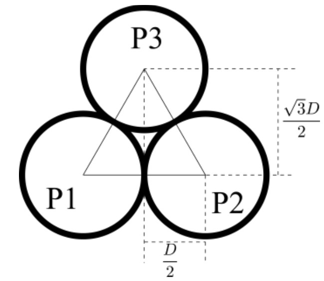
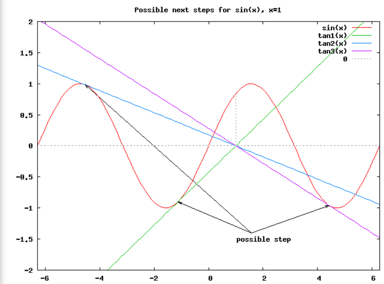
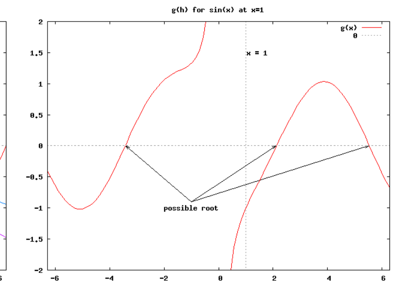
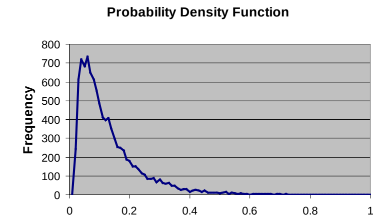
Theory

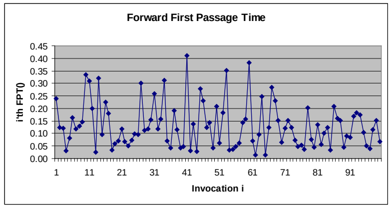
- **New, reversible physical system models**
  - E.g., reversible elastic collisions, phase space coverage
- **Numerical reversal challenges**
  - E.g., reversible transcendental functions
- **Reversible complex probability distributions**
  - E.g., reversible rejection sampling
- **Reversible root-finding**
  - E.g., reversibility of Newton method
- **Other reversible numerical methods**
- **Reversible Turing machines, entropy**

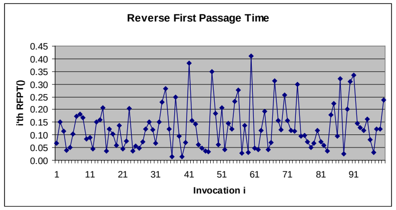







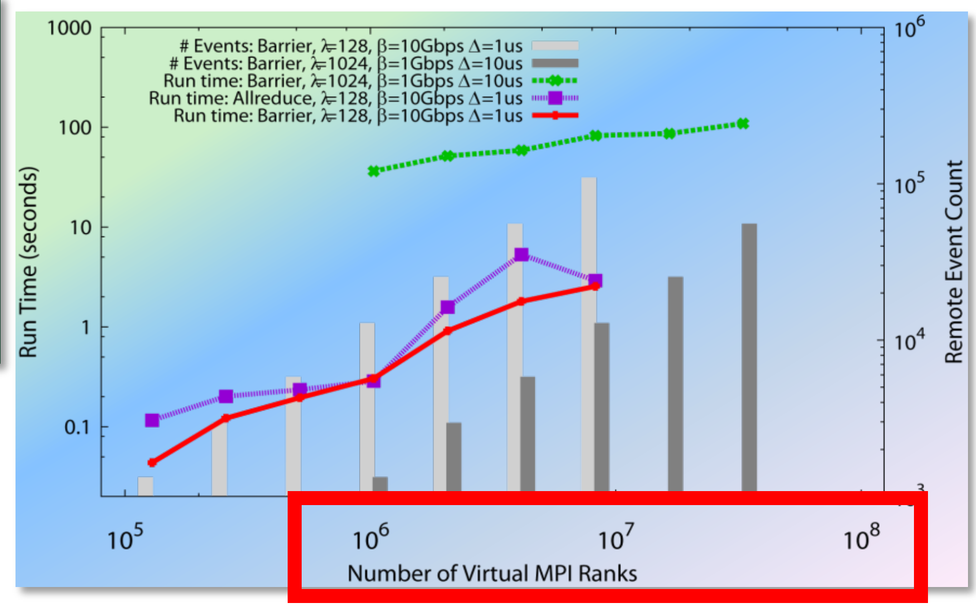




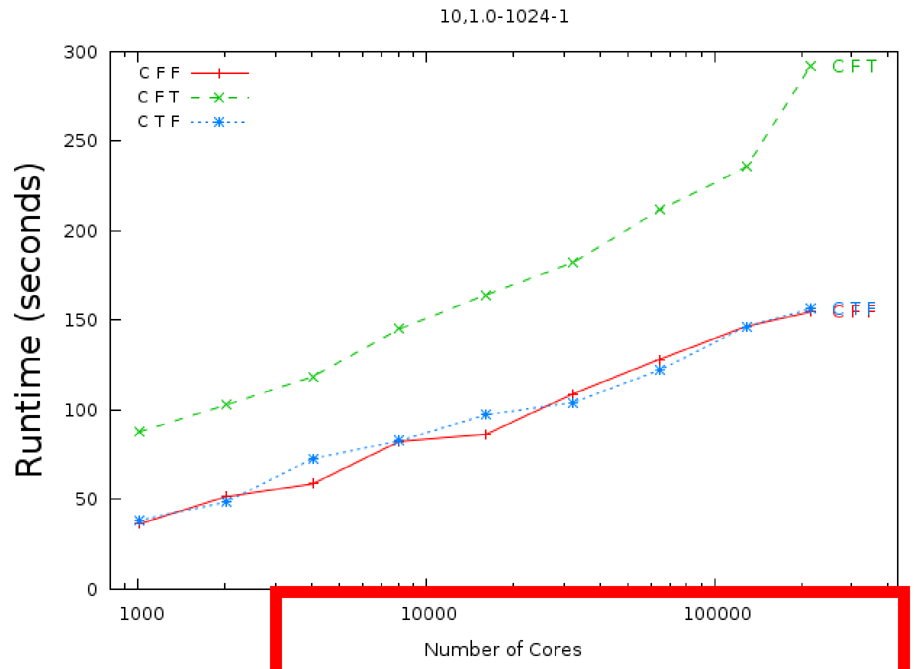


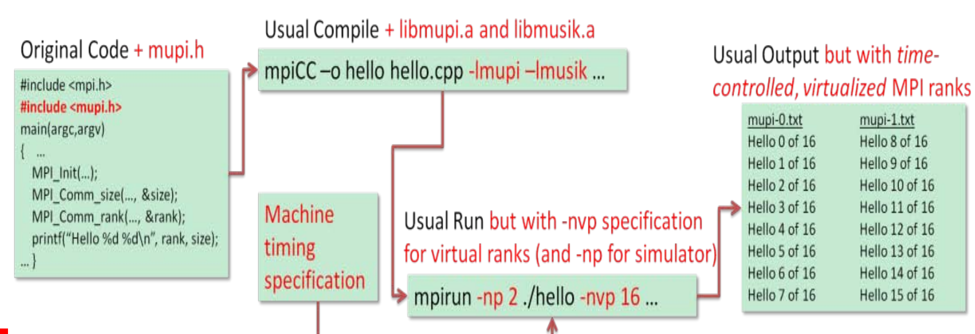
Experimentation – μπ Virtual MPI Testbed 216K Real Cores, 221M Virtual Ranks

- **Facilitates co-design, helps us in experimentation with new runtime frameworks in/over MPI**
- **Several MPI applications tested over μπ**
  - **Tests**: mpiping, allreduce, matmul, pical, …
  - **Benchmarks**: FFTE, GUPS, Gaussian Elimination, …
  - **Applications**: Sweep3D, NWChem, …
  - **DOE Mini-Apps**: pHPCG, CGPOP, …



virtual-barrier, LPX=1024, on Jaguar (Cray XT5)





Experimentation (cont.) – μπ System for Exploring new Million-Rank MPI Runtimes and Applications

What *Challenges*

- **Usable**: Simulate real MPI codes
- **Fast**: Purely discrete event execution
- **Ultra-scale**: 10^6-10^7 ranks
- **Highest fidelity**: Function, timing, feedback

Why *Motivation*

- Exascale co-design
- Prepare software for scaling
- Debug, test, fine-tune frameworks, codes
- Experiment with user-chosen hardware

μπ

Software-based virtual experimentation system

"Seed Corn" of HPC*

How *Techniques*

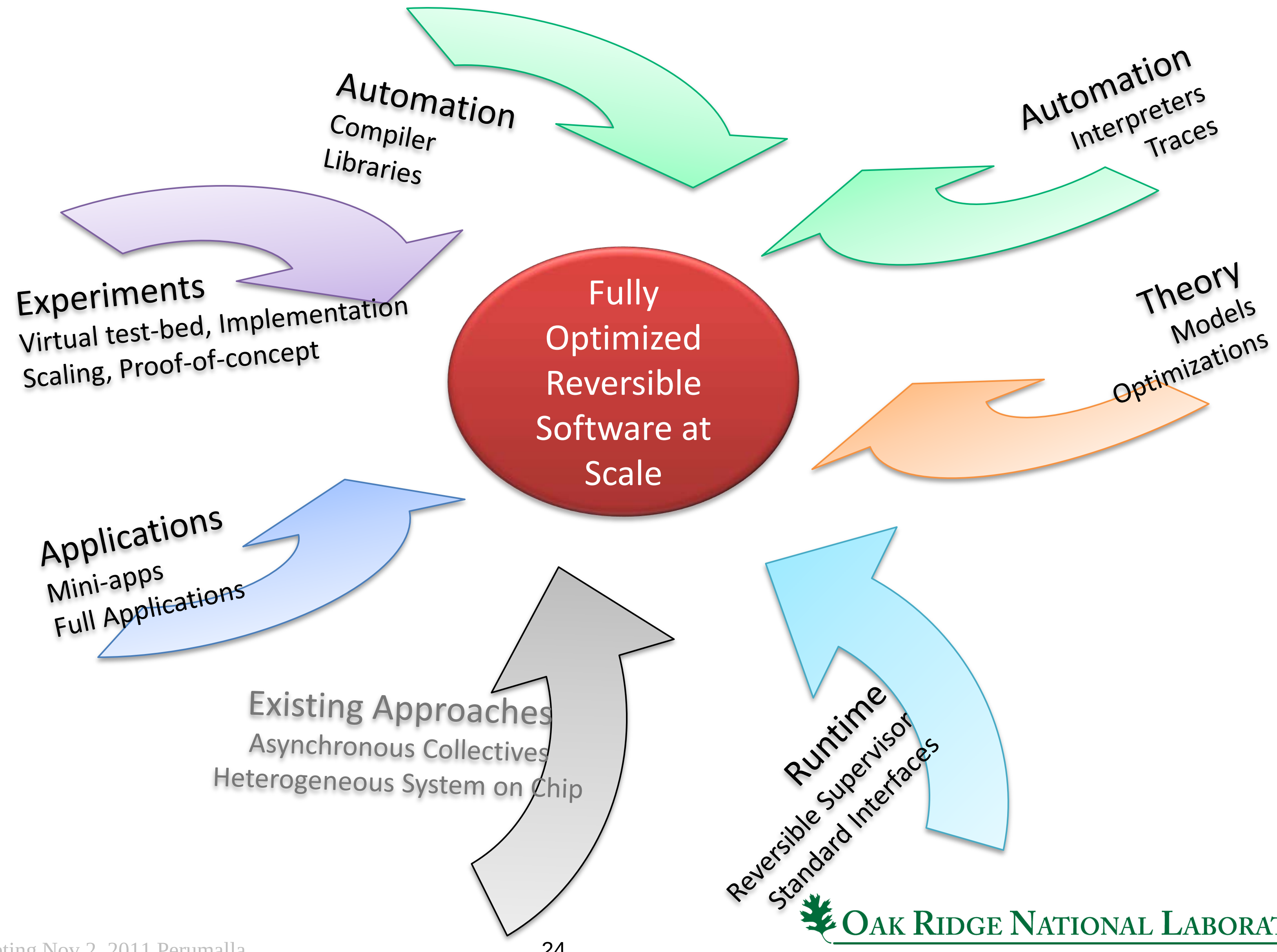
- Multiplex virtual on real ranks
- Optimize virtual MPI layer speed
- Achieve correct timing / ordering
- Expand supported MPI primitives

Etc *Highlights*

- Tested with **several million simulated ranks**
- **1,024 virtual ranks per real rank**
- Tested with multiple MPI benchmarks, apps
- **To be used with DOE mini-apps**

*HPC=High Performance Computing

Vision: Integrated Reversible Software



Outreach – Near-term (Planned)

Software Releases

- Rever-RNG (C, FORTRAN, Java)
- Rever-C (Source-to-Source C Reversal Compiler)
- Rever-BLAS (BLAS extension)
- Rever-Apps (Mini-apps)

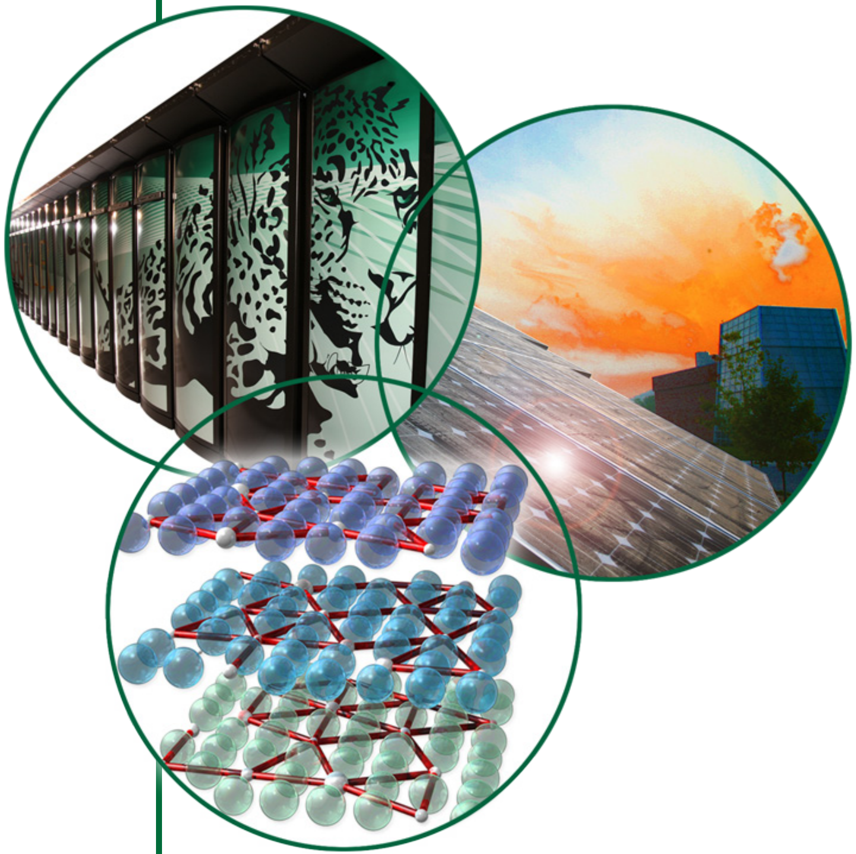
"Rever Challenge Series"

- Competition open to the community
- Easy, medium, hard set of reversal problems
- Reference solutions and implementations to be provided by us at the end of each competition

Summary

- Reversible Software Execution adds an important, orthogonal dimension to high performance computing
- Successful proof-of-concept can jumpstart a new class of research all the way from the top to the bottom layers of HPC
- Technology is in basic research stage
- Challenge is immense but potential payoff for future is high

- Also, positions for future developments
  - Adiabatic Computing, Quantum Computing



Publications

- K. S. Perumalla, A. J. Park and V. Tipparaju, “GVT Algorithms and Discrete Event Execution Dynamics on 129K+ Processor Cores,” International Conference on High Performance Computing, 2011
- K. S. Perumalla and A. J. Park, “Improving Multi-Million Virtual Rank MPI Execution in μπ,“ Intl. Conference on Modeling and Simulation of Computing and Telecommunication Systems, 2011
- S. K. Seal and K. S. Perumalla, “Reversible Parallel Discrete Event Formulation of a TLM-based Radio Signal Propagation Model”, ACM Transactions on Modeling and Computer Simulation, 2011
- K. S. Perumalla and S. K. Seal, “Discrete Event Modeling and Massively Parallel Execution of Epidemic Outbreak Phenomena,” Transactions of the Society for Modeling and Simulation Intl., 2011
- S. K. Seal, K. S. Perumalla and S. P. Hirshman, “Improved Parallelization of the SIESTA Magneto-hydrodynamic Equilibrium Code Using Cyclic Reduction,” DP11 American Physical Society, 2011.
- C. D. Carothers, and K. S. Perumalla, “On Deciding between Conservative and Optimistic Approaches on Massively Parallel Platforms,” Winter Simulation Conference, 2010
- K. S. Perumalla and C. D. Carothers, “Compiler-based Automation Approaches to Reverse Computation,” Workshop on Reverse Computation, 2010
- K. S. Perumalla, “μπ: A Scalable and Transparent System for Simulating MPI Programs,” ICST Intl. Conference on Simulation Tools and Techniques, 2010
- K. S. Perumalla, A. J. Park and V. Tipparaju, “Towards Software-level Virtual Experimentation of MPI-based Million-way Concurrency,” (in preparation)
- K. S. Perumalla and V. A. Protopopescu, “Reversible Simulation of Elastic Collisions,” (in preparation, for Mathematical Modeling in Applied Sciences)

Thank you

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