Sublattice Parallel Replica Dynamics (SLPRD)

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Exascale Computing

From

>HELLO WORLD
>

To

#include <stdio.h>

int main (void)
{
    printf ("Hello, world!");
    return 0;
}
"Big" computers have come a long way since the completion of the Mark I (left) at Harvard in 1944. Capable of approximately three calculations per second, the Mark I was "the first operating machine that could execute long computations automatically," according to IBM. Today, the fastest supercomputer is the Tianhe-2 (right), developed by China’s National University of Defense Technology. The Tianhe-2 has achieved almost 34 petaflops, or 34,000,000,000,000,000 floating-point operations per second.
Scientific Grand Challenges

DISCOVERY IN BASIC ENERGY SCIENCES:
THE ROLE OF COMPUTING AT THE EXTREME SCALE

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- Adaptation to regional climate changes such as sea level rise, drought and flooding, and severe weather patterns;
- Reduction of the carbon footprint of the transportation sector;
- Efficiency and safety of the nuclear energy sector;
- Innovative designs for cost-effective renewable energy resources such as batteries, catalysts, and biofuels;
- Certification of the U.S. nuclear stockpile, life extension programs, and directed stockpile work;
- Design of advanced experimental facilities, such as accelerators, and magnetic and inertial confinement fusion;
- First-principles understanding of the properties of fission and fusion reactions;
- Reverse engineering of the human brain;
- Design, control and manufacture of advanced materials.
The mission and science opportunities in going to exascale are compelling.

For the growing number of problems where experiments are impossible, dangerous, or inordinately costly, extreme-scale computing will enable the solution of vastly more accurate predictive models and the analysis of massive quantities of data, producing quantum advances in areas of science and technology that are essential to DOE and Office of Science missions. For example, exascale computing will push the frontiers of:

- Adaptation to regional climate changes such as sea level rise, drought and flooding, and severe weather patterns;
- Reduction of the carbon footprint of the transportation sector;
- Efficiency and safety of the nuclear energy sector;
- Innovative designs for cost-effective renewable energy resources such as batteries, catalysts, and biofuels;
- Certification of the U.S. nuclear stockpile, life extension programs, and directed stockpile work;
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U.S. economic competitiveness will also be significantly enhanced as companies utilize accelerate development of superior new products and spur creativity arising from modeling and simulation at unprecedented speed and fidelity. An important ingredient is the boost to continued international leadership of the U.S.-based information technology industry at all levels, from laptop to exaflop.
Making the transition to exascale poses numerous unavoidable scientific and technological challenges.

Every major change in computer architecture has led to changes, usually dramatic and often unanticipated, and the move to exascale will be no exception. At the hardware level, feature size in silicon will almost certainly continue to decrease at Moore’s Law pace at least over the next decade. To remain effective in high-end computing systems and in consumer electronics, computer chips must change in radical ways, such as containing 100 times more processing elements than today. Three challenges to be resolved are:

- **Reducing power requirements.** Based on current technology, scaling today’s systems to an exaflop level would consume more than a gigawatt of power, roughly the output of Hoover Dam. Reducing the power requirement by a factor of at least 100 is a challenge for future hardware and software technologies.
- **Coping with run-time errors.** Today’s systems have approximately 500,000 processing elements. By 2020, due to design and power constraints, the clock frequency is unlikely to change, which means that an exascale system will have approximately one billion processing elements. An immediate consequence is that the frequency of errors will increase (possibly by a factor of 1000) while timely identification and correction of errors become much more difficult.
- **Exploiting massive parallelism.** Mathematical models, numerical methods, and software implementations will all need new conceptual and programming paradigms to make effective use of unprecedented levels of concurrency.
Computer Scientist

Researcher

Compiler
Fully atomistic models

- **Classical Molecular Dynamics**
  - Solves Newton equations of motion
    \[ \ddot{r} = -\nabla U + f \]
  - All the physics are included in the empirical potential
  - Extremely parallelizable in space for large systems
  - For small systems the parallel efficiency drops

- **Parallel Replica Dynamics**
  - Parallelizes time evolution
  - Assumptions:
    - Infrequent events
    - Exponential distribution of first-escape times

- **Parareal**
  - Parallelizes time evolution
The properties of the exponential allow us to parallelize time, by having many processors seek the first escape event. The procedure:

- Replicate
- Dephase
- Parallel time
- Allow correlated events

\[ \tau_{\text{corr}} \] (overhead) \rightarrow add all these times together (\( t_{\text{sum}} \)) when first event occurs on any processor

Must detect every transition.

Even with PRD, we have a challenge at the exascale (dephasing overhead dominates for large nproc)

PRD curves assume an average rate of $10^5$ events per atom.second.

Petascale = $10^4$ processors

Exascale = $10^7$ processors

PRD uses 1 proc per replica.
The Exascale Challenge

As the number of processors increases, the Spatially Parallelized Efficiency decreases.

As the number of particles or the number of replicas goes up, the average number of events increases, the PRD Efficiency decreases.

Unreachable part of the exascale triangle
Can we arrange the processors in a different way so to improve the efficiency?

Sublattice PRD (SLPRD)

Speedup:

\[ \eta_{SLPRD} = \frac{N_{PP} \delta(A_R) D}{R \cdot x \cdot t_S} \]

\[ x \cdot t_S \left( 1 + \frac{t_M}{t_B} \right) + \bar{n}_{max} \cdot (t_D + t_C) \]

Spatially Parallelized Efficiency (MD)  
Time Parallelized Efficiency (PRD)

If the number of events is considered a stochastic variable Poisson distributed, the average of the maximum number of events can be calculated analytically

\[ \bar{n} = \sum_n n P_n^{exact} \]

\[ P_n^{exact} = (A + P_n)^D - A^D \]

\[ A = P_0 + P_1 + \cdots + P_{n-1} \]

\[ P_i = \frac{\left( N_{at} k t_{adv} \right)^i}{i!} \cdot \exp\left\{ -N_{at} k t_{adv} \right\} \]
Validation

Checking expression for $\bar{n}_{max}$
- 1 Vacancy in 107 Ni atoms at $T=1022$ K gives an average event rate of $1.07 \times 10^7$ (s atom)$^{-1}$.
- Run dynamics for 2.688 ns.

Checking $\eta$
- 1 Vacancy in 107 Ni atoms at $T=723$ K gives an average rate of $k=10^5$ (s atom)$^{-1}$.
- Run dynamics for 192 ps
- Good agreement between theoretical expressions and simulation results
- Black points for 96 procs and red points for 512 procs
For a large numbers of processors SLPRD becomes more efficient than existing methodologies.
Speedup with the number of atoms

For an intermediate numbers of atoms SLPRD becomes more efficient than existing methodologies
Crossover in efficiency

There is a minimum in the number of processors for a given number of atoms and an average rate.
SLPRD optimum parameters

We can predict the simulation conditions to have optimum scalability
The Exascale Challenge Revisited

SLPRD fills part of the exascale hole
Conclusions

- An increase in computational power will have to come along with new algorithms.
- A strong interaction between researchers and computational scientists will have to be developed in order to take advantage of the new architectures and programming paradigms.