High Performance Algorithms for Scalable Spin-Qubit Circuits with Quantum Dots

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DARPA-QuIST Grant DAAD19-01-1-0659

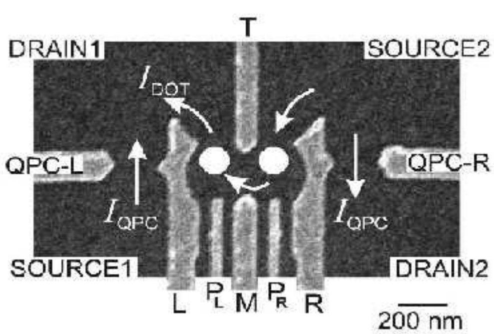
Outline

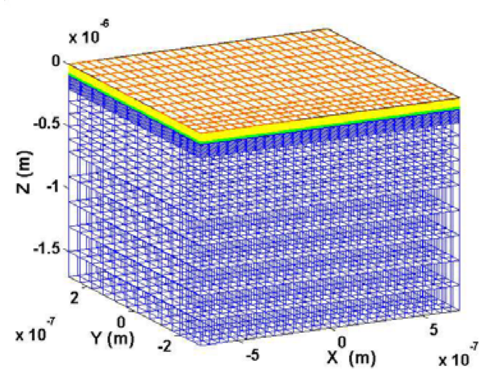
- Description of problem
  - A brief scientific framework
  - Physical and numerical models
- Getting familiar with PETSc
- Computational platforms
- Numerical results
- Conclusions

Scientific Context

- The goal: solid state quantum computers
- Basic information unit: a quantum bit or qubit
    - a physical object that can be represented as a superposition of two basis states in a 2D Hilbert space
    - spin states (**s**) rather than charge-states as qubit
- Need to manipulate the spin **S** of electrons by combining gate electrodes and magnetic fields
- the experimental realization of a solid-state quantum device remains a challenge

Scientific Context





Numerical Model

- 3D self-consistent Poisson–Kohn-Sham scheme
  - Based on the spin-dependent density functional theory (DFT) with local density approximation (LSDA)
  - Well suited to model microscopic quantum many-body phenomena within the device environment
- Electronic states and eigenlevels ϵ of the electron system are obtained by solving Kohn-Sham equations

Numerical Model, continued

- Kohn-Sham equations

$$H^{\uparrow(\downarrow)}\psi^{\uparrow(\downarrow)}(\mathbf{r}) = \epsilon\psi^{\uparrow(\downarrow)}(\mathbf{r})$$

where

$$\begin{aligned} H^{\uparrow(\downarrow)} &= -\frac{\hbar^2}{2}\left[\nabla - \frac{ie}{\hbar c}\mathbf{A}\right]\frac{1}{M}\left[\nabla - \frac{ie}{\hbar c}\mathbf{A}\right] + \\ &+[-e\phi(\mathbf{r}) + \Delta E_c(\mathbf{r}) + \mu_{xc}(\mathbf{r}) + g\mu_B\mathbf{BS}] \end{aligned}$$

- *M* is the electrons mass, **A** is the vector potential corresponding to the uniform magnetic field **B**, *g* and $\mu_B = e\hbar/Mc$ are the Lande factor and effective Bohr magneton, $\mu_{xc}(\mathbf{r})$is the LSDA exchange-correlation potential

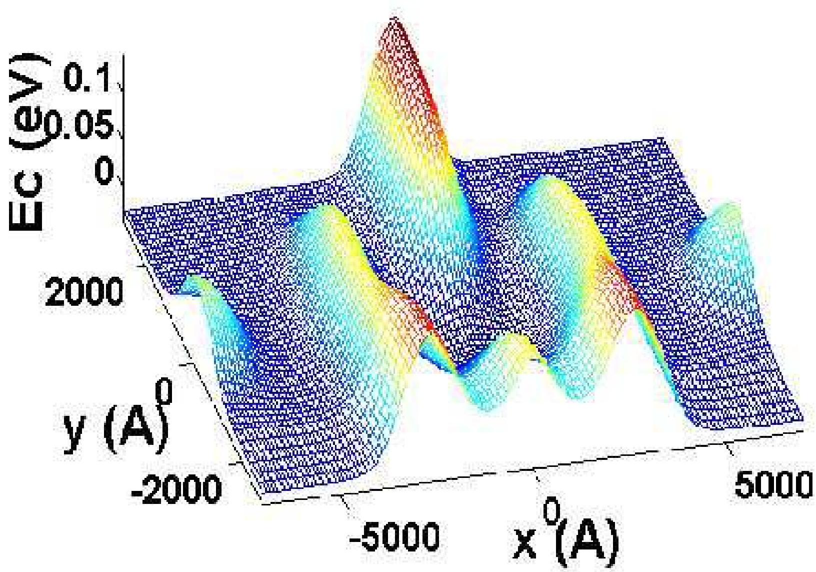
Numerical Model, continued

- $\phi(\mathbf{r})$ is the electrostatic potential determined from the solution of the 3D Poisson equation

$$\nabla\left[\varepsilon(\mathbf{r})\nabla\phi(\mathbf{r})\right] = -\rho(\mathbf{r})$$

- Charge density $\rho(\mathbf{r}) = e\left[p(\mathbf{r}) - n(\mathbf{r}) + N_D^+(\mathbf{r}) - N_A^-(\mathbf{r})\right]$.
- $\varepsilon(\mathbf{r})$ is the permittivity of the material, $p(\mathbf{r})$ is the hole concentration, $n(\mathbf{r})$ the total electron concentration, $N_D^+(\mathbf{r})$, $N_A^-(\mathbf{r})$ are the ionized donor and acceptor concentrations, respectively.

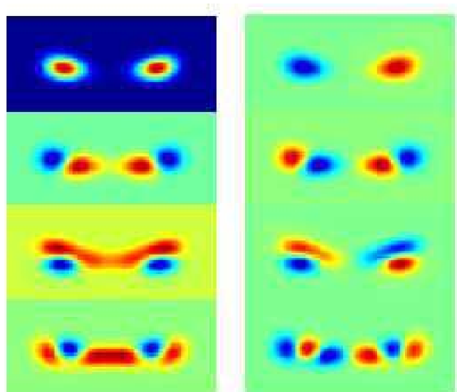
Example Electrostatic Potential



Numerical Model, continued

- The electron concentrations in the quantum dots for each spin are calculated from the wave functions obtained from the Kohn-Sham equations
- The various gate voltages determine the boundary conditions for the Poisson equation.
  - Dirichlet conditions are imposed on the top and bottom surfaces of the structure.
  - For the lateral surfaces vanishing electric fields (von Neumann boundary conditions) or periodic boundary conditions are assumed

Example Wavefunctions



Computational Approach

- The device is mapped onto a 3D non-uniform mesh discretized using the finite element method
  - Must simulate relatively "large" device features ($\sim 0.1\mu$m)
  - Want to resolve nanometer-sized details in quantum dots area
- Newton-Raphson method is used to iteratively solve the self-consistent system of donor charges with the electron charges and spins
- The Kohn-Sham equation is solved using subspace iteration method based on Rayleigh-Ritz analysis

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PETSc

- Portable, Extensible Toolkit for Scientific Computation
  - Nonlinear equations
  - Linear equations
    - Parallel vectors, matrices, mat-vec product
    - Iterative methods and preconditioners
  - Automatic profiling
  - Open source
  - Supported by the authors, petsc-maint@mcs.anl.gov

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How PETSc was used

- `PetscInitialize` and `PetscFinalize`
- Replaced calls to Conjugate Gradient routine
  - Convert matrix and RHS to PETSc formats
  - Call the PETSc solver
  - Obtain solution from PETSc, return as array
- Complications:
  - Solver used for Poisson equation is real-valued
  - Solver used for Kohn-Sham equation is complex-valued

Computational platforms

Tungsten
Linux Cluster
Intel Xeon 3.2 GHz (32-bit)
6.4 Gflops
3 GB per node
Myrinet 2000 interconnect
Linux 2.4.20 (Red Hat 9.0)
1450 (1280 compute nodes)

Computational platforms, continued

Mercury
Linux Cluster
Intel Itanium 2 1.3 or 1.5 GHz (64-bit)
6 Gflops
4 or 12 GB per node
Myrinet 2000 interconnect
Linux 2.4.21-SMP (SuSE Linux SLES8)
631 (1.5 GHz) + 256 (1.3 GHz)

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Computational platforms, continued

Copper
IBM pSeries 690
IBM Power4 1.3 GHz (64-bit)
5.2 Gflops
64 or 256 GB per node
Shared Memory
AIX 5.1
11 32-processor nodes

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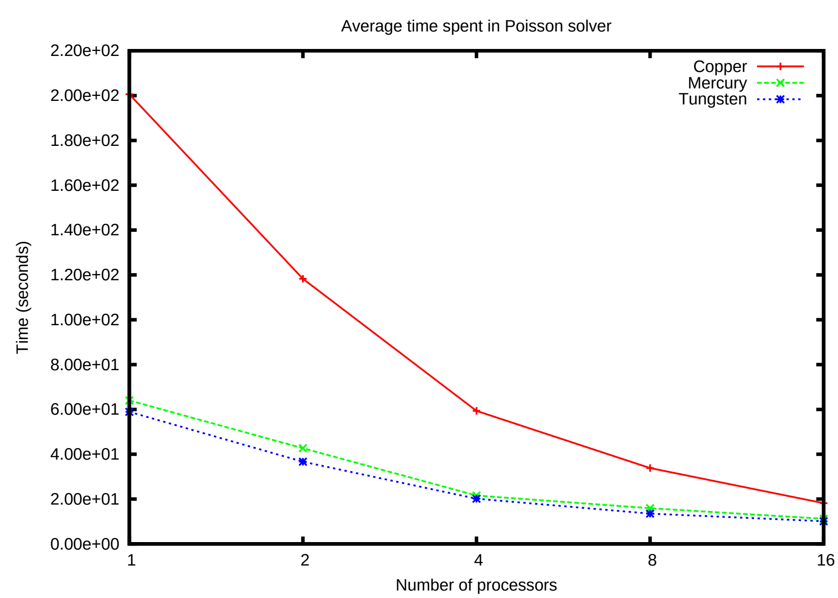
Serial improvement

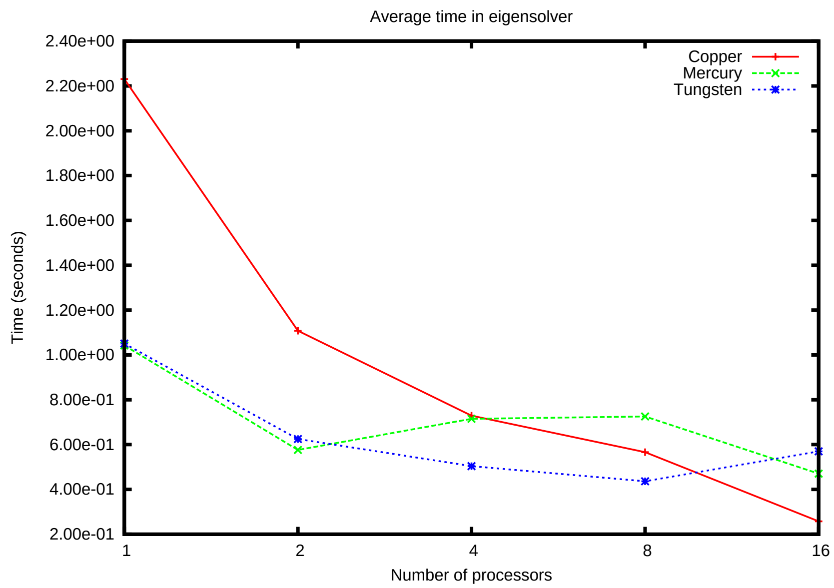
- Comparison between original code and modified one. Calculations are performed on Tungsten.

	Eigenvalue solve	Poisson solve	Total CPU time
Original code	12	90	8430
Improved code	1.10	53.4	4148

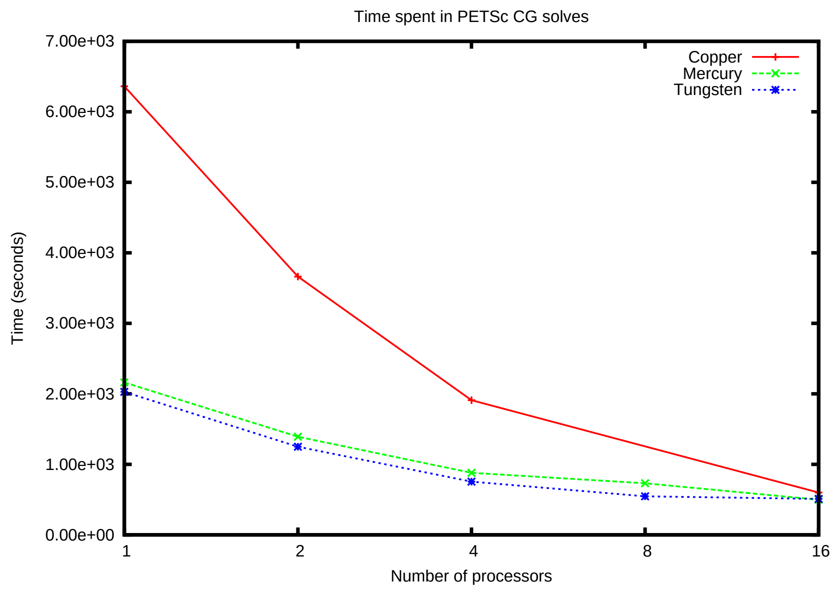
Parallel speedup, Part I



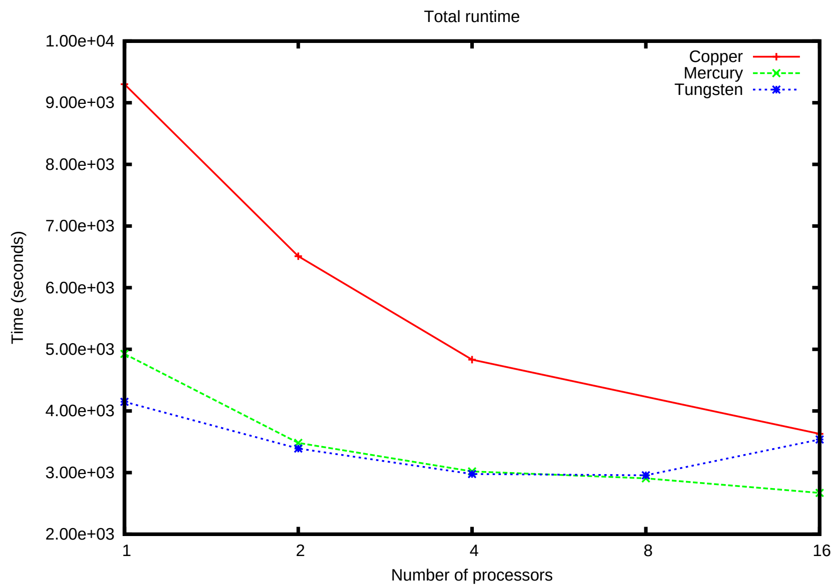
Parallel speedup, Part II



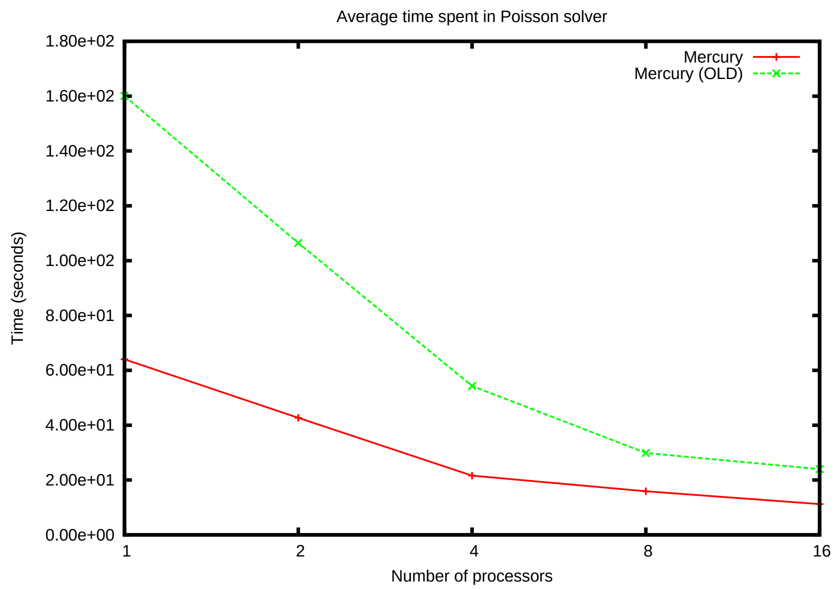
Parallel speedup, Part III



Parallel speedup, Part IV



Mercury improvements



Conclusions

- 10x speedup in the eigenvalue solver in serial
- 2x speedup in the Poisson solver in serial
- Speedup allows for study of a wider range of problems
- Good parallel scaling for problem size
- Would scale farther for larger problems
- Results to be published in the journal Physical Review B