Avenues for Future Research

Avenues for Ongoing/Future Research

- Continuing efforts on linear solvers:
  - Broaden algorithmic and architectural scope of performance studies.
  - Autotuning and composition of linear solvers.
  - Application studies (structures, fluids, nanoscale modeling)
- Linear and non-linear Eigenvalue Problems
- Examine role of emerging language concepts (atomics, transactions) in linear algebra kernels.

Eigenvalue Problems

- Along with linear system solvers, eigenvalue problems are among the most frequently used HPC kernels.

- They are essential to diverse applications in structures, fluids, electromagnetics, nanoelectronics, etc.

Eigenvalue Problems: Example

- Electronic structure calculation requires minimization of the Kohn-Sham (KS) total energy functional associated with an atomistic system with respect to its electron orbitals.

- The total energy can be expressed as:

$$E_{tot}(X) = E_{kin}(X) + E_{ion}(X) + E_H(X) + E_{XC}(X) \qquad (1)$$

  Here $X = (x_1, \ldots, x_k)$ represents the electronic wavefunctions corresponding to k occupied states, and E corresponds to various energy terms.

Eigenvalue Problems: Example

- The total energy must be minimized under the orthonormality constraint $X^T X = I$.

- The Karush-Kuhn-Tucker (KKT) condition yields the following nonlinear eigenvalue problem:

$$H(X)X = X\Lambda_k \tag{2}$$

- $H(X)$ is the Kohn-Sham Hamiltonian that depends on X.

Eigenvalue Problems: Example

- The most commonly used algorithm is the SCF (self consistent field) iteration (fixed point of the KKT condition).
- While the parallelization characteristics of SCF are identical to the linear eigenvalue problem, its convergence is often suspect.
- Other techniques such as direct inversion of iterative subspaces (DIIS) have been proposed to improve robustness.
- While there is some work on parallelization of these schemes, their scaling properties are ill-understood.
- Scaling solutions to this eigenvalue problem to petascale platforms would represent the most significant development in materials modeling.