Enabling Tools for Extreme Scale Computation of Nanoscale Fluids

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Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Overview

- Test several new algorithmic capabilities in Sandia's Tramonto Fluid DFT code
  - Ability to solve fluid-DFT governing equations in 3D and at large scales crucial to continued scientific progress.

- To realize promised performance of modern high-end multicore systems, we must develop new algorithmic capabilities to efficiently utilize multicore nodes
  - Increase performance by reducing node-level memory bandwidth and size usage

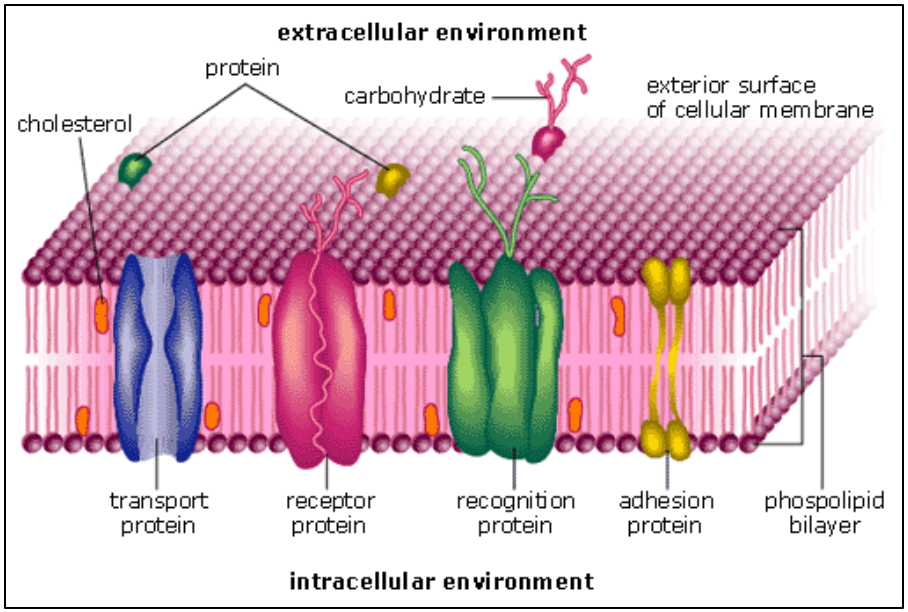
- **Mixed-precision and precision-neutral algorithms**
  - Leverage Trilinos/Tpetra (templated C++) solver stack
  - Performance and storage advantage of float over double
  - Utilize high-precision arithmetic if double inadequate

- **Least-squares methods (LSQR)**
  - Achieve robustness by dynamically adapting precision
  - Shield user from details of mixed-precision computation

- **Block Krylov recycling methods**
  - Recycling subspace information from previous solves to reduce iteration count
  - Block methods have superior convergence properties and computation to bandwidth requirements, improving processor utilization

Nanostructured Fluids

- Structure arises from surfaces, fields, self-assembly
- Density, diffusion, and viscosity different from bulk fluid properties
- Rich phase behavior: wetting, capillary condensation, layering

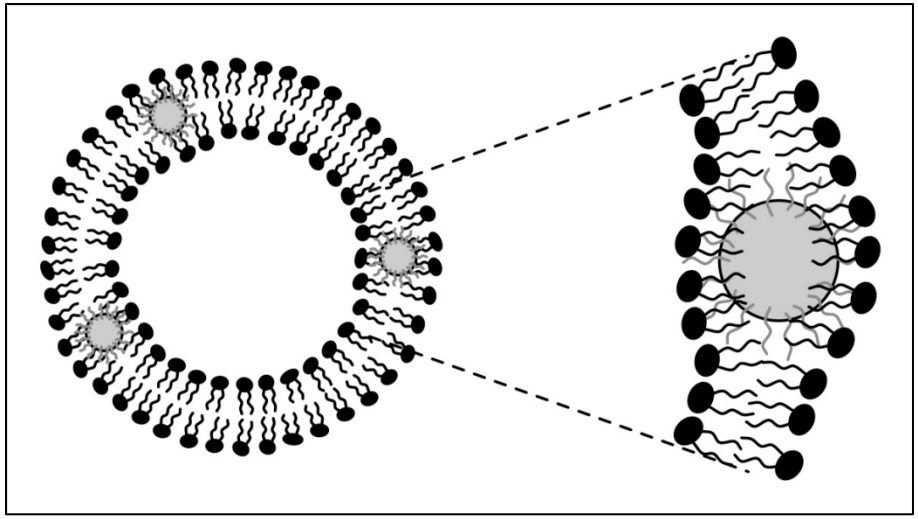


Biological Membranes

Self-assembled fluid bilayer packed with proteins, peptides, etc.

Engineered Systems

Lipid vesicle/nanoparticle assemblies for drug delivery)



[*] G.D. Bothun, Hydrophobic silver nanoparticles trapped in lipid bilayers: Size distribution, bilayer phase behavior, and optical properties, *J. Nanobiotechnology*, 6, (2008).

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Density Functional Theory for Fluids

- Enable modeling and simulation of a wide range of applications, including fluids at interfaces, colloidal fluids, wetting, porous media, and biological mechanisms at the cellular level
- Given external field **V(r)**, determine structure of inhomogeneous fluid as captured by density distribution **ρ(r)** via minimization of free energy functional **Ω(ρ(r))**

Coulomb interactions; Associations (H-bonding); [Applied field]

$$\Omega[\rho(r)] = F_{id} + F_{hs} + F_{vdW} + F_c + F_{assoc} + \int \rho(r)[V(r)-\mu]$$

Ideal gas; Hard sphere; Dispersion attractions

Legendre transform from Canonical to Grand Canonical ensemble

- Solve $\left(\frac{\delta\Omega}{\delta\rho(\mathbf{r})}\right)_{T,\mu} = \mathbf{0}$ with Newton-Krylov.

- Use Sandia's ***Tramonto*** package for complex fluid systems
  - Built upon ***Trilinos*** software components: *trilinos.sandia.gov*
  - Open source: *software.sandia.gov/tramonto/*

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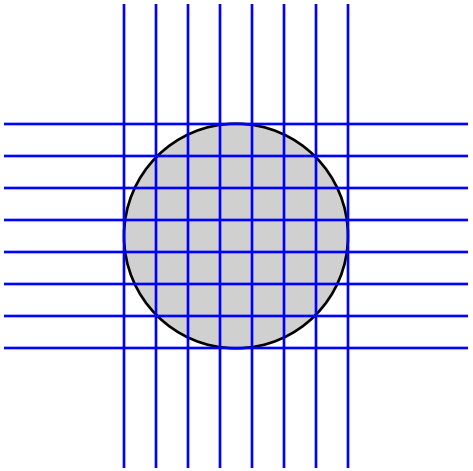
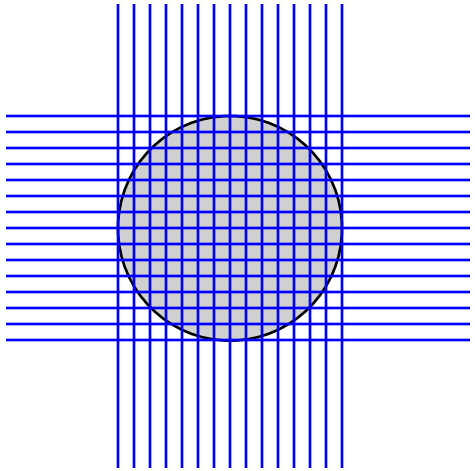
Numerical Methods for Fluid-DFTs

- Discrete formulation
  - Uniform structured grid
  - Discretize using collocation at mesh points
  - Linear interpolation between mesh points
- Newton: Convergence in O(10) iterations
- Linear system properties (different than discrete PDEs)
  - Strong interphysics coupling
  - Large number of DOF/node
  - Nonlocal integral equations
    (matrix sparsity dependent upon mesh)



Coarse Mesh
(Few nonzero per row)



Fine Mesh
(Many nonzero per row)

Segregated Schur Complement Solvers*

- Resulting linear systems take the form

$$\begin{bmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{bmatrix} \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix} = \begin{bmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \end{bmatrix}$$

Each $\mathbf{A}_{ij}$ has own physics-based block structure

- Careful ordering of unknowns makes it advantageous to solve Schur complement

$$\mathbf{S}\mathbf{x}_2 = \mathbf{f}$$

where

$$\mathbf{S} = \mathbf{A}_{22} - \mathbf{A}_{21}\mathbf{A}_{11}^{-1}\mathbf{A}_{12} \qquad \mathbf{f} = \mathbf{b}_2 - \mathbf{A}_{21}\mathbf{A}_{11}^{-1}\mathbf{b}_1$$

- **Schur system may have up to 80% fewer dofs**
- Big win for hard sphere systems: $\mathbf{A}_{11}$ is diagonal!
- Similar favorable structure to $\mathbf{A}_{11}$ for polymer problems using Chandler-McCoy-Singer (CMS) DFT
- More complex structure for WJDC (Werthim, Jain, Dominik, and Chapman) DFT

* M.A. Heroux, A.G. Salinger, and L.J.D. Frink, *Parallel segregated Schur complement methods for fluid density functional theories,* SIAM J. Sci. Comput., 29, (2007). pp. 1526-1535.

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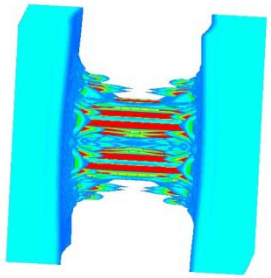
Enabling Mixed-Precision and Precision Neutral Computation

- Rewrite Tramonto solver managers to template scalar, local ordinal, and global ordinal types (templated C++)
  - Arbitrary scalar types: float, complex, dd_real, qd_real **(high precision)**
  - Utilize high-precision arithmetic if double precision inadequate
  - Avoid 4GB limit of int – **allow arbitrarily large problems** (exascale necessity)
  - Enhance performance while maintaining solution accuracy
- **Template scalar type through solver stack**



Fluid-DFT Applications

Tramonto

Fluid DFT Code (C++, Templated)

Scalar Type

Trilinos

Algorithms and Enabling Technologies

Scalar Type

BELOS

Linear Solvers (C++, Templated)

Scalar Type

Tpetra parallel linear algebra library C++, Templated)

Scalar Type

TEUCHOS

Tools Library BLAS/LAPACK wrappers (C++, Templated)

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Precision Neutral Computation

- **Reduce node-level memory bandwidth and size usage**
  - Replace double with float

- Example polymer problem from *Tramonto* (8 linear solves inside Newton loop)

NCore	Float	Double	Speedup
1	3.753	10.970	2.923
2	1.766	4.195	2.375
3	1.203	2.086	1.734
4	1.380	2.643	1.915
5	1.211	2.460	2.031
6	1.056	2.313	2.190
7	1.036	2.057	1.986
8	1.524	2.387	1.566

LSQR

- **LSQR***
  - **Implemented in Trilinos/Belos package (C++, templated)** New!
- Krylov method for **Ax=b** based upon Golub-Kahan bidiagonalization process
- Algebraically equivalent to MINRES applied to normal equations $\mathbf{A^H A x = b}$, but with better numerical properties (especially if **A** ill-conditioned)

- Governing equations

$$\mathbf{A^H U_k = V_k B_k^H} \qquad \mathbf{span(U_k) = \mathcal{K}(AA^H, b)}$$

$$\mathbf{A V_k = U_{k+1} \bar{B}_k} \qquad \mathbf{span(V_k) = \mathcal{K}(A^H A, A^H b)}$$

$$\left\| \mathbf{b - A x_k} \right\| = \min_{\mathbf{y}} \left\| \mathbf{b - A V_k y} \right\| = \min_{\mathbf{y}} \left\| \mathbf{e_1 \beta - \bar{B}_k y} \right\|$$

- **Short-term recurrence; Fixed memory-footprint**
- **Sharp estimates of $\|A\|$, $\|A^{-1}\|$ -> estimate of cond(A)**

- **Robustness under reduced precision**
  - Return least-squares solution to Ax=b even is A numerically singular due to use of lower precision

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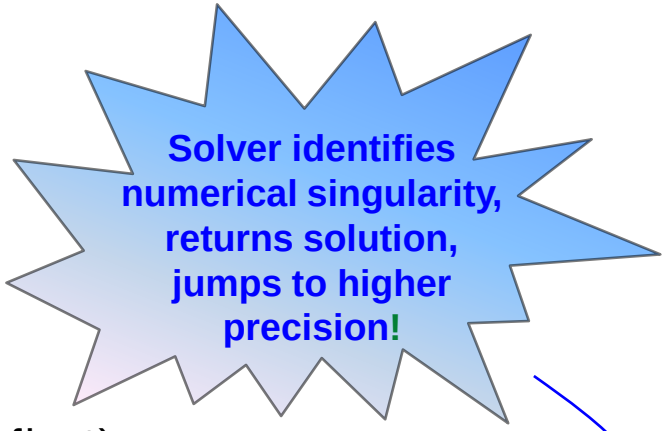
* C. C. Paige and M. A. Saunders, LSQR: An algorithm for sparse linear equations and sparse least squares, TOMS 8(1), 43-71 (1982).

LSQR

- **Balance speed and solution accuracy by dynamically adapting solver precision**
  - (1) Solve Ax=b in float
  - (2) If condest(A) < machEpsSingle return
  - (3) Else solve Ax=b in double
  - (4) If condest(A) < machEpsDouble return
  - (5) Else solve Ax=b in double-double
  - (6) If condest(A) < machEpsDouble-Double return
  - (7) …
- **Shield end user from details of adaptive precision!**
- Adaptive precision example with LSQR
  - Case #1: Well-conditioned matrix (nonsingular in float)
  - Requested relative residual tolerance = 5e-4



Scalar Type	Solve Time (s)	# Iters	CondTest	Residual Norm	Outcome
float	1.049	826	Nonsingular	4.98e-4	Success

  - Case #2: Ill-conditioned matrix (singular in float, nonsingular in double)
  - Requested relative residual tolerance = 1e-6

Scalar Type	Solve Time (s)	# Iters	CondTest	Residual Norm	Outcome
float	8.155	528	Singular	9.80e-6	Failure
double	107.568	4658	Nonsingular	9.99e-7	Success

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Block Recycling Linear Solvers

- Leverage two important algorithmic techniques: **Krylov recycling + block methods**

- **Krylov subspace recycling** ♻
  - In Krylov subspace methods, building search space is dominant cost
  - For sequences of systems, get fast convergence rate and good initial guess immediately by recycling selected search spaces from previous systems
  - Family of recycling methods: Recycling GMRES (GCRODR), recycling CG (RCG), recycling MINRES (RMINRES), recycling BiCG (RBiCG).

- **Block methods**
  - Performance advantages over single-vector methods (BLAS 1 $\rightarrow$ BLAS3, SpMV $\rightarrow$ SpMM)
  - Reduce per-core bandwidth usage
  - Introduce fictitious right-hand-sides to enhance search space

Block Recycling GMRES (BGCRODR)

- **Block Recycling GMRES** New!
  - **Implemented in Trilinos/Belos package (C++, templated)**

(1) Solve $\mathbf{A_1X_1=B_1}$

(2) Compute **k** recycle vectors $\mathbf{U_k}$ (for example, harmonic Ritz vectors)

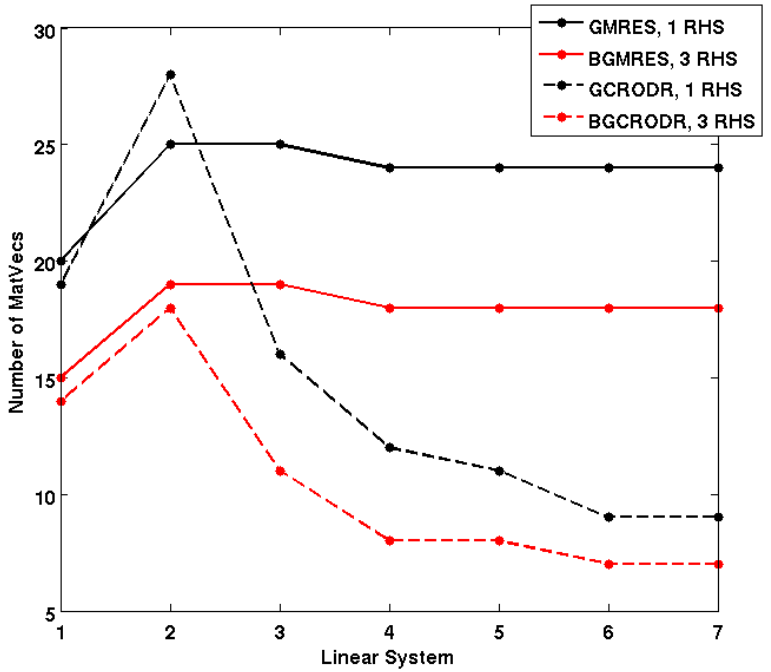
(3) Solve next linear system $\mathbf{A_2X_2=B_2}$ by iterating orthogonally to image of $\mathbf{U_k}$:

$$\mathbf{A_2}\begin{bmatrix}\mathbf{U_k} & \mathbf{W_m}\end{bmatrix}=\begin{bmatrix}\mathbf{C_k} & \mathbf{W_{m+1}}\end{bmatrix}\begin{bmatrix}\mathbf{I_k} & \mathbf{B_k}\\ \mathbf{0} & \underline{\mathbf{H}}_{\mathbf{m}}\end{bmatrix}$$

$$\mathbf{B_k}=\mathbf{C_k^H A W_m} \quad \mathbf{C_k}=\mathbf{A_2U_k} \quad \mathbf{C_k^H C_k}=\mathbf{I_k}$$

(4) Repeat

- Example hard sphere problem from Tramonto (electrostatics + attractions)
- 7 linear solves in from Newton loop
- Savings: 60 matvecs / 36% (1 RHS),
  50 matvecs / 40%, (3 RHS)



BGCRODR on Tramonto Polymer Example

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Summary

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- **Improved performance via reduction of node-level memory bandwidth and size usage**

- **Enabling mixed-precision and precision-neutral algorithms**
  - Leverage Trilinos (templated C++) solver stack
  - 2x or more speedup with float instead of double
  - High-precision arithmetic if double inadequate

- **Least-squares methods (LSQR)**
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- **Block Krylov recycling methods**
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