Electrostatic simulations at Exascale – The beginning of a rusty journey

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Joint with S. Kailasa, M. Scroggs and many other collaborators

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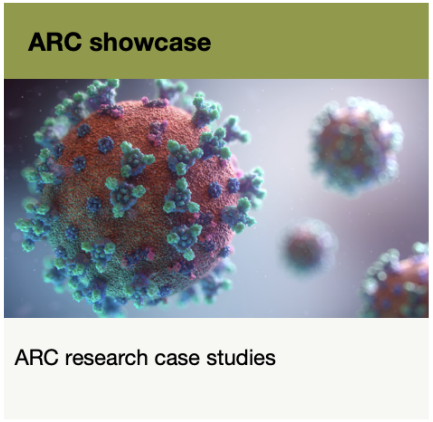
About me



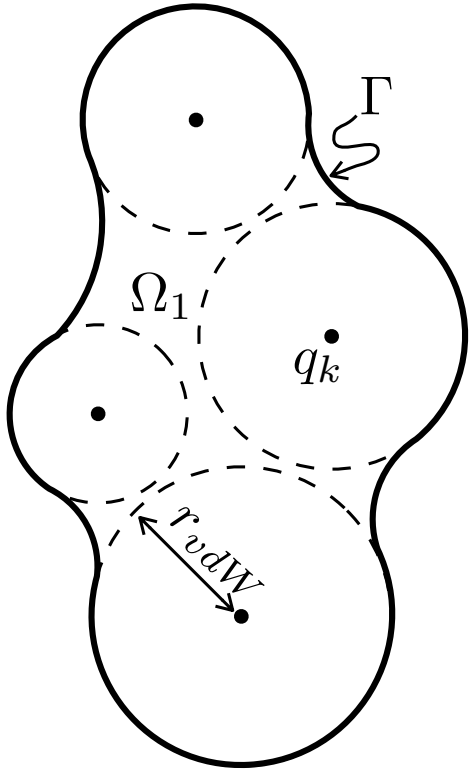
- Professor of Computational Mathematics @UCL Maths
- Associate Director and Director of Research at UCL ARC
- UCL Lead for Excalibur projects on coupling at exascale, and software generation for novel architectures
- Lover of anything Scientific Computing, Rust, and Python

Poisson Boltzmann Models

Poisson-Boltzmann Equation

$$\Delta\phi_1 = \frac{1}{\epsilon_1}\sum_k q_k\delta(\mathbf{r},\mathbf{r}_k) \text{ in } \Omega_1 \quad \Omega_2$$

$$(\Delta - \kappa^2)\phi_2 = 0 \text{ in } \Omega_2$$



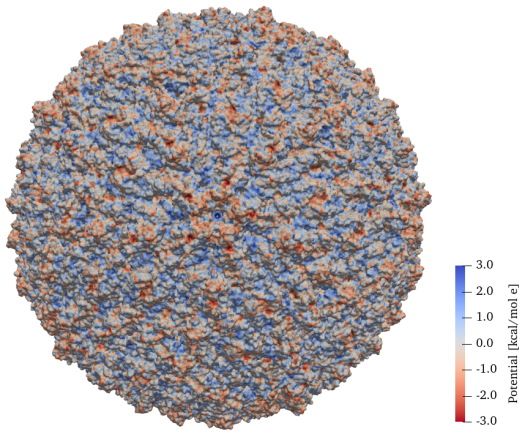
Interface conditions on Γ:

$$\phi_1 = \phi_2,$$
$$\epsilon_1\frac{\partial\phi_1}{\partial\mathbf{n}} = \epsilon_2\frac{\partial\phi_2}{\partial\mathbf{n}}$$

Let $\phi_1 = \phi_{reac} + \phi_{coul}$ (ϕ_{coul} is potential generated from the point charges only). Then want to compute the solvation energy.

$$\Delta G^{polar}_{solv} = \frac{1}{2}\sum_{k=1}^{N_q} q_k\phi_{reac}(\mathbf{r}_k)$$

Exascale FEM/BEM modeling



- Electrostatic simulation of Zika virus (10m elements) on single compute node[1]
- Mass-matrix preconditioned single trace formulation.
- FMM acceleration via ExaFMM.

Goal: Full FEM/BEM modelling of complex protein surfaces.

$$\begin{bmatrix} \epsilon_1 A & -\epsilon_1 M^T \\ \left(\frac{1}{2} I + K\right) & \frac{\epsilon_1}{\epsilon_2} V \end{bmatrix} \begin{bmatrix} \vec{\phi}_1 \\ \vec{\lambda}_2 \end{bmatrix} = \begin{bmatrix} \vec{f} \\ 0 \end{bmatrix}.$$

A: FEM matrix, K: Double-Layer operator, V: Single-Layer operator, M: Mass matrix

Want to scale up to billions surface dofs.

[1] T. Wang, C. D. Cooper, T. Betcke, L. A. Barba, *High-productivity, high-performance workflow for virus-scale electrostatic simulations with Bempp-Exafmm*, submitted (2021)

Software Technologies

Python

- Good for higher level logic.
- Efficient libs for array processing.
- Performance for complex algorithms in Python (e.g. FMM) difficult[2].

Python + Code Gen

- Most flexible solution.
- Complex framework.
- What low-level language to use?

C++

- Complex Makefiles.
- Deployment difficult.
- C++20 support still patchy.

[2] S. Kailas et. al., *PyExaFMM: an exercise in designing high-performance software with Python and Numba*, to be submitted

Scientific computing with Rust

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- Modern language design.
- Great tooling.
- Compile time safety guarantees.
- Simple deployment.
- Python integration trivial.

Design a set of libraries in Rust that can be easily composed into large parallel FEM/BEM applications.

The Rust Scientific Computing ecosystem

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Core utilities

- Num - Traits and utility routines for floating point types.
- Cauchy - A complex scalar type library (uses Num).
- approx - Unit test routines for floating point types.
- Serde - Serialization library.

Linear Algebra/Machine Learning

- ndarray - multidimensional array type in Rust.
- nalgebra - Rust linear algebra library with Lapack bindings.
- householder - Early stages linear algebra library.
- Linfa - Native machine learning in Rust.
- tensorflow - Rust bindings to tensorflow.
- petsc-rs - Rust bindings for Petsc.

Parallelization

- rsmpi - MPI Interface for Rust.
- Rayon - Fork/Join threading, parallel loops and iterators.
- async/await (Tokio, etc.) - frameworks for asynchroneous execution.

Language bindings

- PyO3 - Binding complex Rust types to Python.
- maturin - Simple tools to wrap Rust C API bindings with Python cffi.
- Any language that supports C bindings can talk to Rust easily.

Still lots of moving parts in the ecosystem but an enormous amount of development happening.

What makes Rust great for HPC?

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- Fully built on top of LLVM.
- Strong and rich type system with traits based generics resolved at compile time.
- All type conversions must be explicit (no accidental assignment of a 64 bit integer to a 32 bit variable).
- Very simple foreign function interface to integrate existing C code without overhead.
- Simple but powerful error handling.

...However, CUDA support still very early stages (but OpenCL works well)

Example: A new approach to large scale linear algebra

- Joint work with Jed Brown (Colorado Boulder)
- Design traits (and prototype implementations) that provide a unified approach to linear algebra in finite and infinite dimensional spaces
- Currently implementing minimum viable product
- Want to have a modern Rust native sparse linear algebra kernel

Novel unified linear algebra traits

```rust
// A base operator trait.
6 implementations
pub trait OperatorBase: Debug {
    type Domain: LinearSpace;
    type Range: LinearSpace;

    /// Returns a reference to trait object that supports application of the operator.
    ///
    /// By default it returns an `Err`. But for concrete types
    /// that support matvecs it is specialised to return
    /// a dynamic reference.
    fn as_apply(&self) -> Option<&dyn AsApply<Domain = Self::Domain, Range = Self::Range>> {
        None
    }

    fn has_apply(&self) -> bool {
        self.as_apply().is_some()
    }
}
```

```rust
/// Definition of a linear space
///
/// Linear spaces are basic objects that can create
/// elements of the space.
6 implementations
pub trait LinearSpace {
    /// Field Type.
    type F: Scalar;

    /// Type associated with elements of the space.
    type E<'b>: Element<Space = Self>
    where
        Self: 'b;

    /// Create a new vector from the space.
    fn create_element<'b>(&'b self) -> Self::E<'b> {
        std::unimplemented!();
    }
}
```

- Use subtraits to model normed spaces, inner product spaces, etc.
- Can build iterative solvers on top of traits without knowledge of underlying implementation

Early stage Rust solver infrastructure

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tree	Fast distributed octree management
grid	Distributed parallel grids
element	Tabulation and evaluation of finite elements
green-kernel	Direct evaluation of Green's functions
quadrature	Collection of quadrature rules
fmm	Distributed fast multipole methods

- Using Python + JIT (e.g. Numba) works well for simple array oriented algorithms. More problematic for complex algorithms.
- We are at the start of a multi-year journey to develop very large-scale integral equation solvers in Rust.
- Rust is ready for scientific computing and allows us to rethink how to design modern computational libraries.