Productive Performance Portability: Building in Rust with PETSc and libCEED

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Overview

Rust for HPC

- Rust provides high performance with modern tooling and ergonomic language features
- We look at the libCEED and PETSc Rust wrappers
- The libCEED wrapper provides performance portable matrix-free finite element operators
- The PETSc wrapper is a more complex ongoing challenge

Rust is ready for HPC - but it requires rethinking your design!

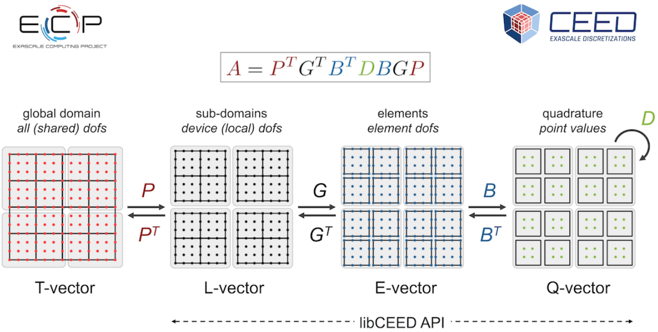
Rust - Language features

- Strongly typed language with a focus on performance and safety
- Compile-time memory management via lifetimes
- Borrow checker protects data, tracking ownership and access
- Many C run-time bugs become Rust compile-time errors

Rust - Ergonomics

- Installing - Cargo + crates.io manages dependencies vs Make
- Abstractions - zero cost abstractions for high-level language features
- Documentation - Automatic documentation with doctests using Cargo + docs.rs
- Unit Tests - Doctests and unit tests integrated with Cargo

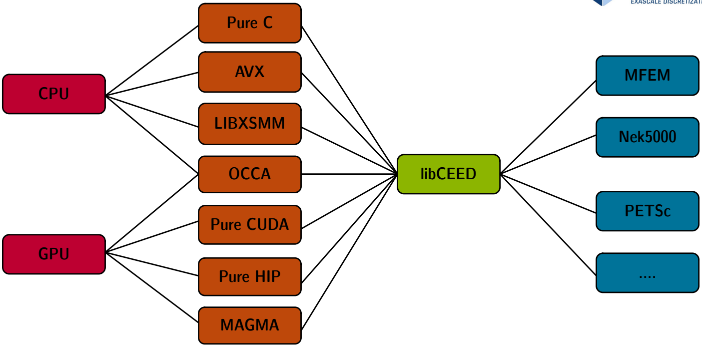
libCEED Representation



[2]

- **P** - parallel element assembly operator
- **G** - local element assembly operator
- **B** - basis action operator
- **D** - weak form and geometry at quadrature points

libCEED Backends



[2]

Multiple backends provide performance portability at runtime

Rust wrapper preserves this capabilty (mostly)!

libceed-rs

https://lib.rs/crates/libceed
https://github.com/ceed/libceed

- Faithful translation of C API into Rust
- Additional objects to help manage borrowed vector access
- Currently no native Rust GPU QFunction support

```rust
extern crate libceed;
fn main() -> libceed::Result<()> {
    let ceed = libceed::Ceed::init("/cpu/self/ref");
    let u = ceed.vector_from_slice(&[0.0, 0.5, 1.0])?;
    let u_view = u.view()?;
    assert_eq!(u_view[..], [0.0, 0.5, 1.0]);
    Ok(())
}
```

Building

Building dependencies reliabily across platforms can be... painful

```
...

ifneq ($(wildcard $(XSMM_DIR)/lib/libxsmm.*),)
  PKG_LIBS += -L$(abspath $(XSMM_DIR))/lib -lxsmm -ldl
  MKL ?=
  ifeq (,$(MKL)$(MKLROOT))
    BLAS_LIB = -lblas
  else
    ifneq ($(MKLROOT),)
      # Some installs put everything inside subdirectory
      MKL_LIBDIR = $(dir $(firstword $(wildcard $(MKLROOT)/lib/intel64/libmkl_sequentia
      MKL_LINK = -L$(MKL_LIBDIR)
      PKG_LIB_DIRS += $(MKL_LIBDIR)
    endif
    BLAS_LIB = $(MKL_LINK) -Wl,--push-state,--no-as-needed -lmkl_intel_lp64 -lm
  endif
  PKG_LIBS += $(BLAS_LIB)
endif
...
```

Building

Far simpler dependency specification for Rust!

```toml
[package]
name = "ex1-volume"
version = "0.1.0"
authors = [
    "Jeremy L Thompson <thompson.jeremy.luke@gmail.com>",
]
edition = "2018"

[dependencies]
libceed = "0.9.0"
structopt = { version = "0.3", default-features = false }
mesh = { path = "../mesh" }
```

Easier building

```
$ cargo build
```

High Level Abstractions - User QFunctions

User source for physics at quadrature points requires some additional boilerplate in C/CUDA single source

```
CEED_QFUNCTION(MassApply)(void *ctx, const CeedInt Q,
                          const CeedScalar *const *in,
                          CeedScalar *const *out) {
  // Unpack input and output arrays
  const CeedScalar *u = in[0], *rho = in[1];
  CeedScalar *v = out[0];

  // Loop over all quadrature points
  CeedPragmaSIMD
  for (CeedInt i = 0; i < Q; i++) {
    v[i] = u[i] * rho[i];
  }

  return 0;
}
```

High Level Abstractions - User QFunctions

Rust inteface presents more clarity, less opportunity for error

```
// QFunction from user closure
let apply_mass = |
    [u, qdata, ..]: QFunctionInputs,
    [v, ..]: QFunctionOutputs,
| {
    // Protected array access!
    v.iter_mut()
        .zip(u.iter().zip(qdata.iter()))
        .for_each(|(v, (u, rho))| *v = u * rho);

    0
};
```

Documentation

Documentation and testing separate in C
Often multiple processing steps to generate documentation

```c
/**
  @brief Create a CeedVector of the specified length
             (does not allocate memory)

  @param       ceed   Ceed context
  @param       length Length of vector
  @param[out]  vec    Address where the newly created
                        CeedVector will be stored

  @return An error code: 0 - success, otherwise - failure

  @ref User
**/
int CeedVectorCreate(Ceed ceed, CeedInt length,
                     CeedVector *vec) { /* */ };
```

Documentation

Integrated documentation and unit tests in Rust

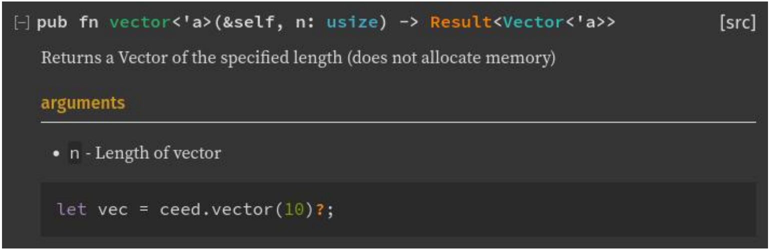
```
/// Returns a Vector of the specified length
///   (does not allocate memory)
///
/// # arguments
///
/// * ‘n‘ - Length of vector
///
/// ‘‘‘
/// # use libceed::prelude::*;
/// # fn main() -> libceed::Result<()> {
/// # let ceed = libceed::Ceed::default_init();
/// let vec = ceed.vector(10)?;
/// # Ok(())
/// # }
/// ‘‘‘
pub fn vector<’a>(&self, n: usize) -> Result<Vector<’a>> { /* */ }
```

Documentation

Easier testing and documentation

```
$ cargo test
$ cargo fmt
$ cargo doc
```

Automatically tested code snippits in documentation examples



```
[-] pub fn vector<'a>(&self, n: usize) -> Result<Vector<'a>>        [src]
```

Returns a Vector of the specified length (does not allocate memory)

arguments

- `n` - Length of vector

```
let vec = ceed.vector(10)?;
```

Lost in Translation

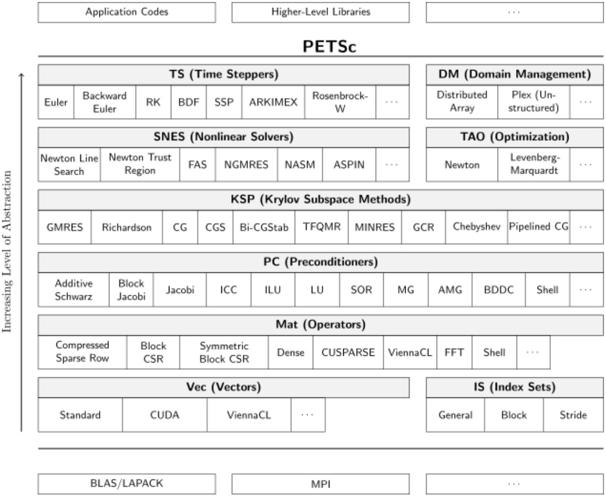
Passive vectors can be mutated by operators

```
// Mass operator
let qf_mass = ceed.q_function_interior_by_name("MassApply")?;
let op_mass = ceed
      .operator(&qf_mass, QFunctionOpt::None, QFunctionOpt::None)?
      .field("u", &ru, &bu, VectorOpt::Active)?
      .field("qdata", &rq, BasisOpt::Collocated, &qdata)?
      .field("v", &ru, &bu, VectorOpt::Active)?
      .check()?;

v.set_value(0.0)?;
op_mass.apply(&u, &mut v)?;
```

If `"qdata"` was an output, the operator could mutate the underlying data without the Rust compiler knowing

PETSc - the Portable, Extensible Toolkit for Scientific Computation



[1]

petsc-rs

https://lib.rs/crates/petsc
https://gitlab.com/petsc/petsc-rs

- Attempt to maintain flexibility of C API
- Wider range of additional objects to manage borrowed access
- Currently incomplete shell object support

High Level Abstractions - Matrix assembly

```rust
let n = 5;
let mut mat = petsc.mat_create()?;
mat.set_sizes(None, None, n as usize, n as usize)?;
mat.set_from_options()?;
mat.set_up()?;

// Stencil (-1, 2, -1)
let v = [Scalar::from(-1.0), Scalar::from(2.0), Scalar::from(-1.0)];
mat.assemble_with_batched(
    (0..n)
        .map(|i| {
            if i == 0 { ([i], [-1, i, i + 1], &v) }
            else if i == n - 1 { ([i], [i - 1, i, -1], &v) }
            else { ([i], [i - 1, i, i + 1], &v) }
        }),
    InsertMode::INSERT_VALUES,
    MatAssemblyType::MAT_FINAL_ASSEMBLY,
)?;
```

Lost in Translation - Part II

- PETSc objects have bi-directional data ownership
- Compiler can't reliably reason about complex lifetimes
- The libCEED wrapper provides performance portable matrix-free finite element operators
- The PETSc wrapper is a more complex ongoing challenge

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Future Work

- Expand PETSc Rust wappers
- Native Rust libCEED QFunctions for GPU
- PETSc + libCEED Rust examples
- Clarify inner mutability vs interface level mutability across FFI barrier
- Disentangling object lifetimes

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Satish Balay, Shrirang Abhyankar, Mark F Adams, Jed Brown, Peter Brune, Kris Buschelman, Lisandro Dalcin, Alp Dener, Victor Eijkhout, William D Gropp, Dmitry Karpeyev, Dinesh Kaushik, Matthew G Knepley, Dave A May, Lois Curfman McInnes, Richard Tran Mills, Todd Munson, Karl Rupp, Patrick Sanan, Barry F Smith, Stefano Zampini, Hong Zhang, and Hong Zhang.
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