Parallel workflows for computational science and engineering: FEniCS (draft)

Architecture, interfaces and syntax

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Aims/Vision of FEniCS

- Research setting:
  - Adaptive general FEM/HPC software for PDE: FEniCS
  - Focus on challenging problems in turbulence/fluid-structure interaction
- Automated computational modeling: weak form of PDE as input + tolerance on output quantity ⇒ automated generation of discretization and solution satisfying tolerance
  - Automated weak form evaluation/tensor assembly
  - Automated duality-based error control/adaptivity
  - Automated modeling: no explicit turbulence model, turbulent dissipation comes only from numerical stabilization
  - Optimal strong scaling up to thousands of cores for full framework on massively parallel hardware

FEniCS development

FEniCS:

`fenicsproject.org` Open source software project for automated solution of PDE with many involved universities/individuals. (see `fenicsproject.org` for developer info/papers).
Python and C++ programming interface.

FEniCS-HPC:

Branch with focus on good scaling on massively parallel architectures, targeting open/challenging problems in turbulent flow/FSI. Developed mainly by CTL group.
Only the C++ programming interface.

`fenicsproject.org`
`ctl.csc.kth.se`

The Finite Element Method (notation)

Want to solve differential equation:
$R(u) = 0$ or
$(R(u), v) = \int_\Omega R(u) v dx = 0, \forall v \in V$ (weak/variational form)

We seek a solution U in finite element vector space V^h defined by the mesh and basis functions ϕ_j of the form:

$$U(x) = \sum_{j=1}^{M} \xi_j \phi_j(x)$$

We require the residual to be orthogonal to V^h:

$$(R(U), v) = 0, \forall v \in V^h$$

Typical notation for linear problems:
$(R(U), v) = a(U, v) - L(v) = 0$
Ex. Poisson:
$R(u) = \Delta u - f = 0, \quad a(U, v) - L(v) = (\nabla U, \nabla v) - (f, v) = 0$

FEniCS main concepts

1. Functions and function spaces
2. Form language (expressions of Functions)
3. Forms (weak formulation of PDE)
4. Assembling tensors (matrix/vector/scalars)
5. Solving linear systems
6. Boundary conditions
7. Automated linearization

Architecture of FEniCS

Component structure:

- Automated generation of finite elements/basis functions (FIAT)

$$e = (K, P, \mathcal{N})$$

- Automated evaluation of variational forms on one cell based on code generation (FFC+UFL)

$$A^K = a_K(v, U) = \int_K \nabla v \cdot \nabla U dx$$

- Automated assembly of discrete systems on a mesh $\mathcal{T}_\Omega$ (DOLFIN-HPC)

```
$A = 0$
for all elements $K \in \mathcal{T}_\Omega$
    $A$ += $A^K$
```

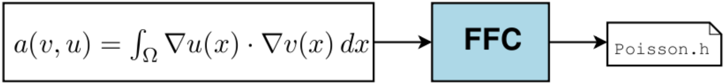
- Automated turbulent Unified Continuum modeling (Unicorn)

$$r_{UC}(v, W) = (v, \rho(\partial_t u + (u \cdot \nabla)u) + \nabla \cdot \sigma - g) + SD(v, W)$$

FEniCS form compilation/code generation

- Automates a key step in the implementation of finite element methods for partial differential equations

- Input: a variational form and a finite element
- Output: C/C++ function for element tensor



$a(v,u) = \int_\Omega \nabla u(x) \cdot \nabla v(x)\, dx$

FFC

`Poisson.h`

Input form in (ASCII) mathematical notation:

```
a = inner(grad(v), grad(u))*dx
```

Compiler:

```
>> ffc [-l language] poisson.form
```

Generated quadrature code

```
virtual void tabulate_tensor(double* A, const double* const* w,
     const ufc::cell& c) const
{
...
  // Quadrature weight
  const static double W0 = 0.5;
  // Tabulated basis functions and arrays of non-zero columns
const static double Psi_w[1][3] =\
  {{0.33333333333, 0.33333333333, 0.33333333333}};
 const static double Psi_vu[1][2] = {{-1, 1}};
 static const unsigned int nzc0[2] = {0, 1};
 static const unsigned int nzc1[2] = {0, 2};
 // Geometry constants
 const double G0 = Jinv_00*Jinv_10*W0*det;
 const double G1 = Jinv_01*Jinv_11*W0*det;
 const double G2 = Jinv_00*Jinv_00*W0*det;
 const double G3 = Jinv_01*Jinv_01*W0*det;
 const double G4 = Jinv_10*Jinv_10*W0*det;
 const double G5 = Jinv_11*Jinv_11*W0*det;
 // Loop integration points
 for (unsigned int ip = 0; ip < 1; ip++)
 {
   // Compute function value
   double F0 = 0;
   for (unsigned int r = 0; r < 3; r++)
     F0 += Psi_w[ip][r]*w[0][r];
   const double Gip0 = (G0 + G1)*F0;
   const double Gip1 = (G2 + G3)*F0;
   const double Gip2 = (G4 + G5)*F0;
   for (unsigned int i = 0; i < 2; i++)
   {
     for (unsigned int j = 0; j < 2; j++)
     {
       A[nzc0[i]*3 + nzc0[j]] += Psi_vu[ip][i]*Psi_vu[ip][j]*Gip1;
       A[nzc0[i]*3 + nzc1[j]] += Psi_vu[ip][i]*Psi_vu[ip][j]*Gip0;
       A[nzc1[i]*3 + nzc0[j]] += Psi_vu[ip][i]*Psi_vu[ip][j]*Gip0;
       A[nzc1[i]*3 + nzc1[j]] += Psi_vu[ip][i]*Psi_vu[ip][j]*Gip2;
     }
   }
 }
}
```

Stokes equation: form language

$$\begin{aligned} -\Delta u + \nabla p &= f \\ \nabla \cdot u &= 0 \end{aligned}$$

```
# Create mixed space (Taylor-Hood)
V = VectorElement(``Lagrange'', ``tetrahedron'', 2)
Q = FiniteElement(``Lagrange'', ``tetrahedron'', 1)
TH = V * Q

# Create trial and test functions
(u, p) = TrialFunctions(TH)
(v, q) = TestFunctions(TH)

# Coefficient function appearing in L
f = Coefficient(V)

# Define forms
a = inner(grad(u), grad(v))*dx - p*div(v)*dx + div(u)*q*dx
L = dot(f, v)*dx

# Compute solution w = (u, p) with BCs given in ``bcs''
w = Function(TH)
solve(a == L, w, bcs)
```

Functions and function spaces (Python)

Import the DOLFIN Python interface:

```
from dolfin import *
```

Load mesh and create cG(1) function space (continuous piecewise linear functions):

```
mesh = UnitSquare(5, 5)
V = FunctionSpace(mesh, "CG", 1)
```

Create a function $U \in V$ and inspect the vector of coefficients ξ:

```
U = Function(V)
print U.vector().array()
```

Alternatively load a mesh from file:

```
mesh = Mesh("mesh.xml")
```

Expressions (known coefficients)

Represent the known coefficient $f(x) = cos(3) * x_0$ with $x = [x_0, x_1]$ in 2D.

```
f = Expression("cos(3)*x[0]")
```

Function expressions

Differential and algebraic operators in text-version of mathematical notation (example: $q = \nabla U \cdot \nabla U - fU$):

```
q = inner(grad(U), grad(U)) - f*U
```

See the UFL manual for full syntax.

Form notation (weak formulation of PDE)

Recall notation of inner product:
$M = \|\nabla U\|^2 = (\nabla U, \nabla U) = \int_\Omega \nabla U \cdot \nabla U dx$

In FEniCS:

```
M = inner(grad(U), grad(U))*dx
```

Also possible to express boundary terms, here $M = \int_\Gamma U ds$:

```
M = U*ds
```

Form notation (weak formulation of PDE)

Recall how we defined the weak form of a PDE:
$a(U, v) = L(v), \forall v \in V_h$

For Poisson's equation for example:
$(\nabla U, \nabla v) = (f, v), \forall v \in V_h$

Introduce two special functions:

```
U = TrialFunction(V) # Unknown function we seek
v = TestFunction(V) # All functions in V
```

We can now express the above *bilinear form* $a(U, v)$ and *linear form* $L(v)$ like so:

```
a = inner(grad(U), grad(v))*dx
L = f*v*dx
```

Assembling tensors (matrix/vector/scalar)

A bilinear form $a(U, v)$ corresponds to a matrix $A_{ij} = a(\phi_i, \phi_j)$.
A linear form $L(v)$ corresponds to a vector $b_i = L(\phi_i j$
A functional M corresponds to a scalar $q = M$

We can assemble a form into the corresponding tensor by:

```
A = assemble(a)
b = assemble(L)
q = assemble(M)
```

For example, assembling the L_2-norm of a function: $\|f\| = \sqrt{(f, f)}$

```
M = inner(f, f)*dx
f_L2norm = assemble(M)
f_L2norm = sqrt(f_L2norm)
```

Solving linear systems

FEniCS has a high-level interface to state-of-the-art linear algebra packages (PETSc, Trilinos, etc.)

To solve a linear system with the default linear solver:

```
x = Vector()
solve(A, x, b)
```

We can also use the compact solve interface for the PDE:

```
U = Function(V)
solve(a == L, U)
```

with the possibility of choosing different solvers and options:

```
solve(a == L, U, solver_parameters= \
 {‘‘linear_solver’’: ‘‘bicgstab’’, \
  ‘‘preconditioner’’: ‘‘ilu’’}
```

Boundary conditions

…

Complete basic FEniCS Poisson demo

```
from dolfin import *

# Create mesh and define function space
mesh = UnitSquare(32, 32)
V = FunctionSpace(mesh, "CG", 1)

# Define Dirichlet boundary (x = 0 or x = 1)
def boundary(x):
    return x[0] < DOLFIN_EPS or x[0] > 1.0 - DOLFIN_EPS

# Define boundary condition
u0 = Constant(0.0)
bc = DirichletBC(V, u0, boundary)

# Define variational problem
v = TestFunction(V)
u = TrialFunction(V)
f = Expression("10*exp(-(pow(x[0]␣-␣0.5,␣2)␣+␣pow(x[1]␣-␣0.5,␣2))␣/␣0.02)")
g = Expression("sin(5*x[0])")
a = inner(grad(v), grad(u))*dx
L = v*f*dx - v*g*ds

# Compute solution (assemble matrix/vector, solve linear system)
U = Function(Vh)
solve(a == L, U, bcs=bc)

# Plot solution
plot(u, interactive=True)
```

Automated linearization

…

Hands-on demonstration

Complete goal-oriented adaptive solver

Exercise

Worksheet: Adaptive stabilized Navier-Stokes