PETSc TAO support for optimisation problems with FEniCSx

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18 June 2025 | FEniCS'25 conference

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Optimisation Problems

$$\min_x f(x)$$

Optimisation Problems

Let $f : \mathbb{R}^n \to \mathbb{R}$

$$\min_{x \in \mathbb{R}^n} \quad f(x)$$

- Unconstrained

Optimisation Problems

Let $f : \mathbb{R}^n \to \mathbb{R}$, $x^-, x^+ \in \overline{\mathbb{R}}^n$

$$\begin{aligned} \min_{x \in \mathbb{R}^n} \quad & f(x) \\ \text{subject to} \quad & x^- \leq x \leq x^+ \end{aligned}$$

- Unconstrained
- Bound constrained

Optimisation Problems

Let $f : \mathbb{R}^n \to \mathbb{R}$, $x^-, x^+ \in \overline{\mathbb{R}}^n$, $g : \mathbb{R}^n \to \mathbb{R}^m$ and $h : \mathbb{R}^n \to \mathbb{R}^l$.

$$
\begin{aligned}
\min_{x \in \mathbb{R}^n} \quad & f(x) \\
\text{subject to} \quad & x^- \leq x \leq x^+ \\
& g(x) = 0 \\
& h(x) \geq 0
\end{aligned}
$$

- Unconstrained
- Bound constrained
- General constrained

Optimisation Problems

Let $f : \mathbb{R}^n \to \mathbb{R}$, $x^-, x^+ \in \overline{\mathbb{R}}^n$, $g : \mathbb{R}^n \to \mathbb{R}^m$ and $h : \mathbb{R}^n \to \mathbb{R}^l$.

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- Unconstrained
- Bound constrained
- General constrained

$\to$ PETSc's **T**oolkit for **A**dvanced **O**ptimization (TAO) [1]

Optimisation Problems over Function Spaces

$$\begin{aligned} \min_{x \in \mathbb{R}^n} \quad & f(x) \\ \text{subject to} \quad & x^- \le x \le x^+ \\ & g(x) = 0 \\ & h(x) \ge 0 \end{aligned}$$

Optimisation Problems over Function Spaces

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$$\begin{aligned} \min_{u \in V} \quad & f(u) \\ \text{subject to} \quad & u^- \le u \le u^+ \\ & g(u) = 0 \\ & h(u) \ge 0 \end{aligned}$$

Motivation

- Non abstraction breaking
- Automatic differentiation, form manipulation, ... – `ufl`
- Uniform interface for un-, bound- or general constrained problems
- Multi field
- Optional abstractions

Previous Work

- Bound constrained, single field, no automatic differentiation
  - `FreeFem++` [2]
  - `comet-fenicsx` [3]
- SNES solver, blocked systems, `ufl`
  - `dolfiny` [4]
  - `DOLFINx` [5]
- Variational inequality solvers with SNES VI
  - `MFEM` [6]
  - `Firedrake` [7]
- Convex optimisation with `MOSEK`, multi field, `ufl`
  - `dolfinx_optim` [8]

```python
from dolfiny.taoproblem import TAOProblem
```

A Poisson Solver

We consider

$$-\Delta u = f \quad \text{in } \Omega = (0,1)^2$$
$$u = g \quad \text{on } \partial\Omega$$

as energy minimisation problem

$$\min_{\substack{u \in H^1(\Omega) \\ u|_{\partial\Omega}=g}} \frac{1}{2}\int_\Omega \nabla u^2 \, \mathrm{d}x - \int_\Omega f u \, \mathrm{d}x.$$

```python
from dolfinx import fem, mesh
from dolfiny.taoproblem import TAOProblem

domain = mesh.create_unit_square(
  MPI.COMM_WORLD, 32, 32
)
V = fem.functionspace(domain, ("P", 1))

u = fem.Function(V)
F = (
  .5 * ufl.inner(ufl.grad(u), ufl.grad(u)) * ufl.dx
  - f * u * ufl.dx
)
bc = fem.dirichletbc(g, facet_dofs, V)

opts = PETSc.Options("poisson")
opts["tao_type"] = "bqnls"
opts["tao_ls_type"] = "armijo"
opts["tao_max_it"] = 300
opts["tao_gttol"] = 1e-5

tao = TAOProblem(F, [u], bcs=[bc], prefix="poisson")
tao.solve()
```

But, SNES can line search

- Both TAO and SNES search for a stationary point

$$\delta f(u^\star) = R(u^\star) = 0.$$

- For a descent direction p, line search computes step size

$$\alpha = \operatorname*{argmin}_{\hat{\alpha}>0} f(u + \hat{\alpha} p).$$

- SNES will use (by default)

$$f(u) = ||R(u)||_2^2.$$

  - Dangerous – not respecting discretization.

Poisson with Bound Constraints

We consider

$$-\Delta u = f \quad \text{in } \Omega = (0,1)^2$$
$$u = g \quad \text{on } \partial\Omega$$

as energy minimisation problem

$$\min_{u \in H^1(\Omega)} \frac{1}{2} \int_\Omega \nabla u^2 \,\mathrm{d}x - \int_\Omega f u \,\mathrm{d}x$$

subject to $\quad g - \iota_{\partial\Omega} \leq u \leq g + \iota_{\partial\Omega},$

where $\iota_{\partial\Omega} = \begin{cases} 0 & x \in \partial\Omega \\ \infty & \text{else.} \end{cases}$

```
u = fem.Function(V)
F = (
  .5 * ufl.inner(ufl.grad(u), ufl.grad(u)) * ufl.dx
  - f * u * ufl.dx
)

lb = fem.Function(V)
lb.interpolate(
  lambda x: np.where(
    np.isclose(x[0], 0) or np.isclose(x[0], 1) or
    np.isclose(x[1], 0) or np.isclose(x[1], 1),
    g,
    np.full(x.shape[1], -np.inf),
  )
)

ub = fem.Function(V)
ub.interpolate(...)

opts = PETSc.Options()
opts["tao_type"] = "bnls"
opts["tao_ls_type"] = "unit"
opts["tao_gatol"] = 1e-14

tao = TAOProblem(F, [u], ub=[ub], lb=[lb])
tao.solve()
```

Optimal Control

We consider

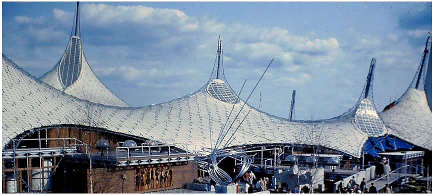
$$\min_{f \in H^1(\Omega)} ||u_d - u(f)||_{L^2}^2 + \frac{\alpha}{2} ||f||_{L^2}^2$$

where $u(f)$ is the solution of

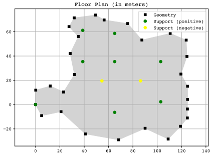
$$\begin{aligned} -\Delta u &= f \quad \text{in } \Omega = (0,1)^2 \\ u &= g \quad \text{on } \partial\Omega. \end{aligned}$$

```python
from dolfiny.taoproblem import sync_functions

state_problem = fem.petsc.LinearProblem(...)
adjoint_problem = fem.petsc.LinearProblem(...)

@sync_functions(f)
def F_hat(tao, x):
    state_problem.solve()
    return comm.allreduce(fem.assemble_scalar(F))

@sync_functions(f)
def J_hat(tao, x, J):
    state_problem.solve()

    adjoint_problem.solve()

    # jacobian = p + alpha * f
    jacobian.x.array[:] = (
        p.x.array[:] + alpha * f.x.array[:]
    )
    fem.petsc.assign(jacobian, J)

tao = TAOProblem(
    F_hat, [f], J=(J_hat, f.x.petsc_vec.copy())
)
tao.solve()
```

German Pavilion Expo ’67



German Pavilion at Expo ’67 in Montreal [9].

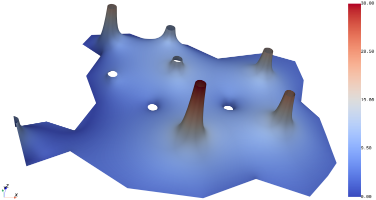


Floor plan of the Pavilion geometry [11].

$$\min_{\substack{g\in H^1(\Omega)\\ g|_{\partial\Omega}=h}} \int_\Omega \sqrt{|\nabla g|^2+1}\,\mathrm{d}x + \alpha||g||^2_{H^1}$$

subject to $\quad \phi \le u \le \psi.$

- For *smooth* h, ϕ and ψ this is well-posed [10].



Computed surface $\{(x, y, g(x, y)) \mid (x, y) \in \Omega\}$.

Truss Sizing Optimisation

$\Omega \subset \mathbb{R}^3$ truss structure [12]

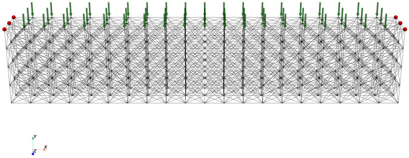
$$\min_{s \in DG_0(\Omega)} \int_{v \in \Gamma_f} u(s) \cdot f \, \mathrm{d}P$$

subject to $s_{\text{min}} \leq s \leq s_{\text{max}}$

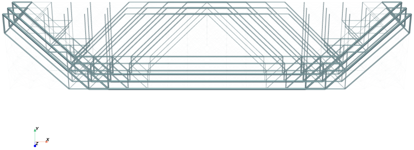
$$\int_\Omega s \, \mathrm{d}x = \frac{1}{20} \int_\Omega s_{\text{max}} \, \mathrm{d}x,$$

where $u(s) \in P_1(\Omega)$ solves

$$\int_\Omega s\sigma(u)\varepsilon(v) \, \mathrm{d}x = \int_{v \in \Gamma_f} f \cdot v \, \mathrm{d}x \quad \forall v.$$



Truss geometry $100 \times 20 \times 10\, m$.



Optimised truss structure, radii scaled by factor 5.

Experience with PETSc TAO

- Python TAO interface sparsely used
  - `GitHub` search for `PETSc.TAO()` yields 70 results
  - Routines for general constrained problems previously not exported
- Unconstrained and bound constrained problems – *just work*
- General constrained problems – *not battle tested*
  - `ALMM` is the only usable general constrained solver – Bugs identified
  - `PDIPM` does not support ghosted vectors – `IPOPT` [13] contender?

Outlook

- NEST matrices
- Multiple constraint support
- Further applications in shape- and topology optimisation
- Custom optimiser through PETSc Python interface
- Automatic reduced functional – pyadjoint-x? [14]

dolfiny.uni.lu

fenics-dolfiny/dolfiny

pip install dolfiny

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