Los Alamos NATIONAL LABORATORY

What can PyNumero do for me?
A tutorial

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May 8, 2025

LA-UR-25-24472

Roadmap

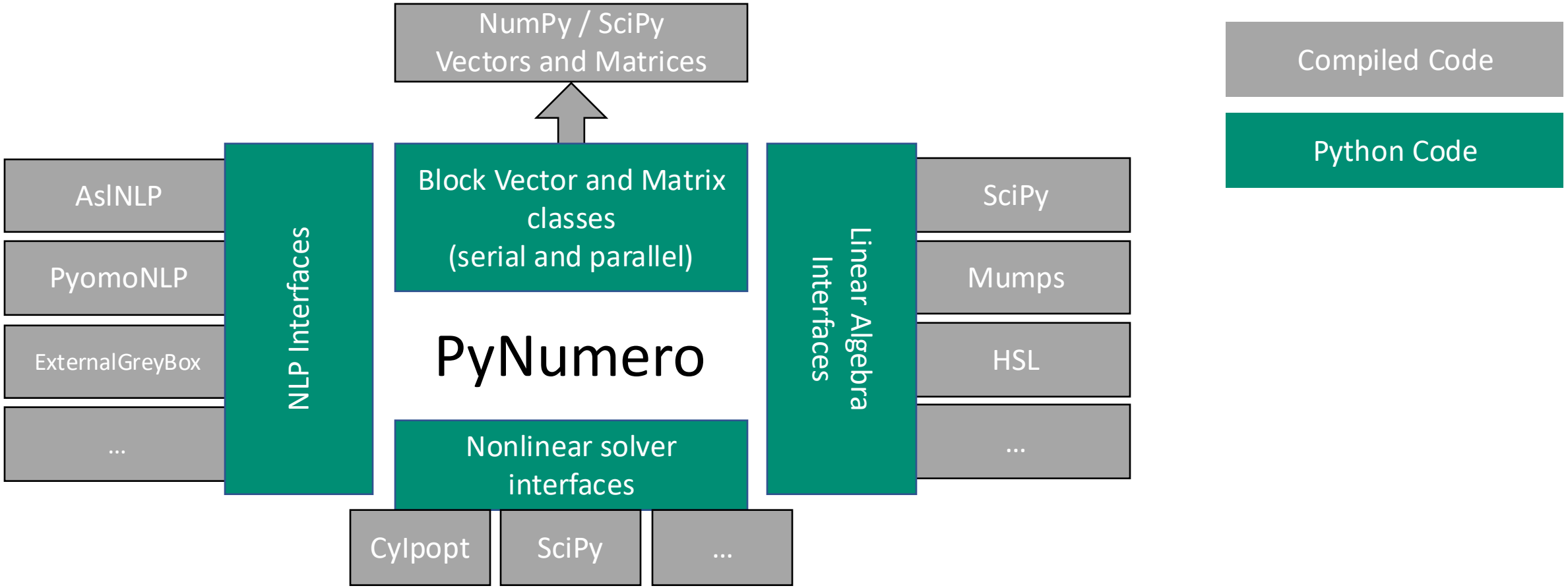
1. What is PyNumero?

2. What can PyNumero do for me? (Examples)

3. What can I do for PyNumero? (Ideas for future developers)

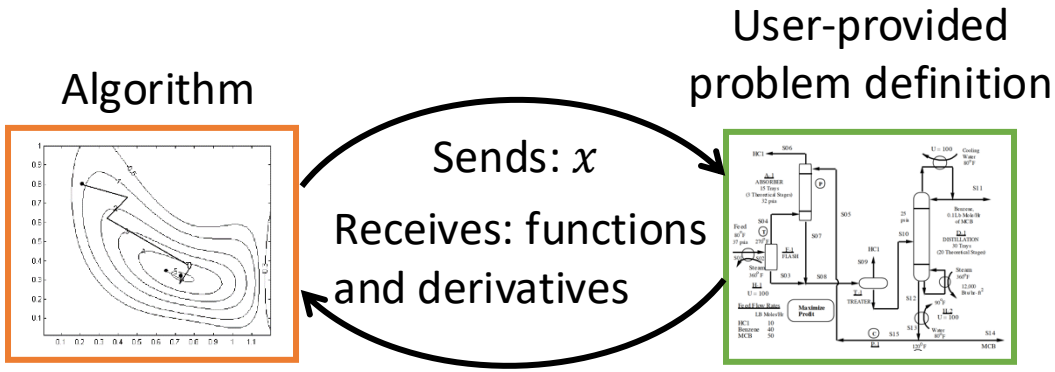
What is PyNumero?

Interfaces to libraries for automatic differentiation, matrix factorization, and parallelization.

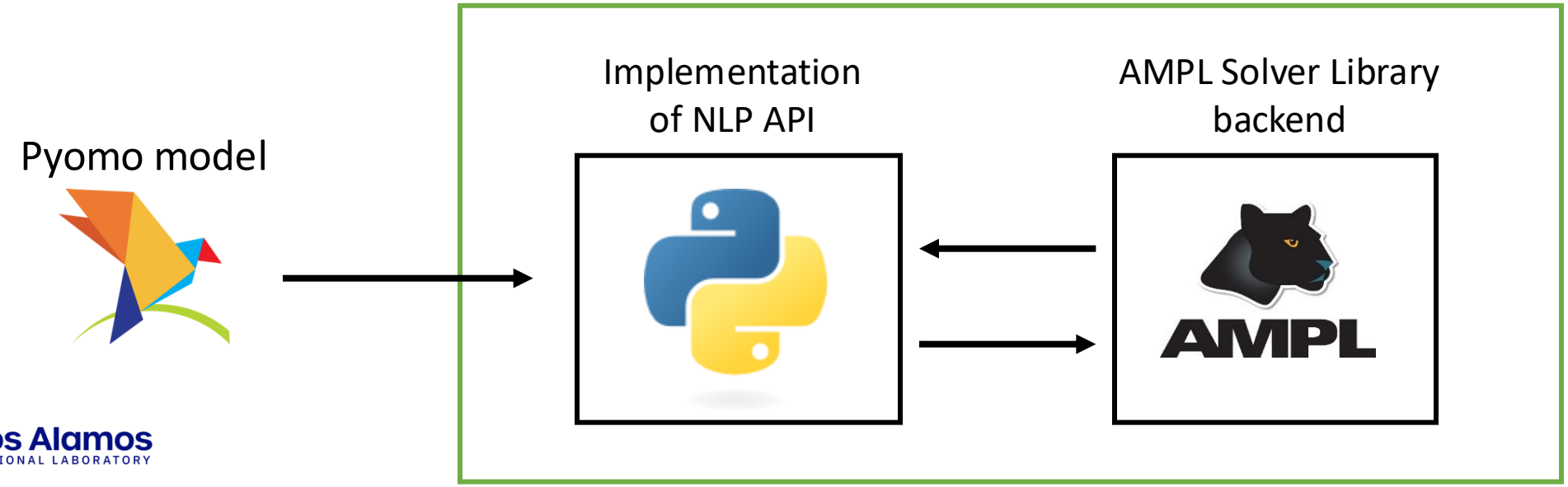


NLP interfaces implement the callbacks that NLP solvers require

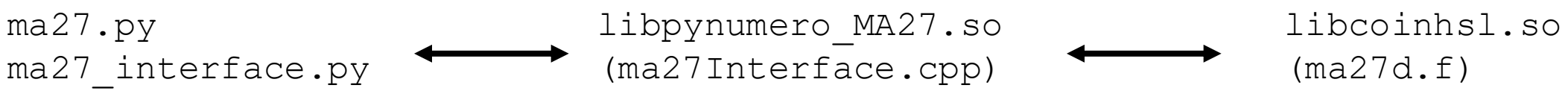
$$\begin{aligned} \min_{x} \quad & \varphi(x) \\ \text{s.t.} \quad & f(x) = R \\ & L \leq g(x) \leq U \\ & x^L \leq x \leq x^U \end{aligned}$$



In practice:



Linear solver interfaces wrap MA27, MA57, and MUMPS for use in custom algorithms



Can wrap these interfaces (again) for a particular application, e.g., an interior point method.

PyNumero contains solver interfaces that utilize the NLP API

```
pyo.SolverFactory("cyipopt")
pyo.SolverFactory("scipy.fsolve")
```

Advantages:

- Can solve custom NLP objects
- Access to solver callbacks

What can PyNumero do for me?

1. Inspect your reduced Hessian
2. Track metrics during a solve
3. ~~Solve a model with user-defined functions~~

The reduced Hessian is an important part of NLP algorithms and optimality conditions

$$\begin{aligned} \min_{x} \quad & \varphi(x) \\ \text{s.t.} \quad & f(x) = 0 \\ & g(x) \leq 0 \end{aligned}$$

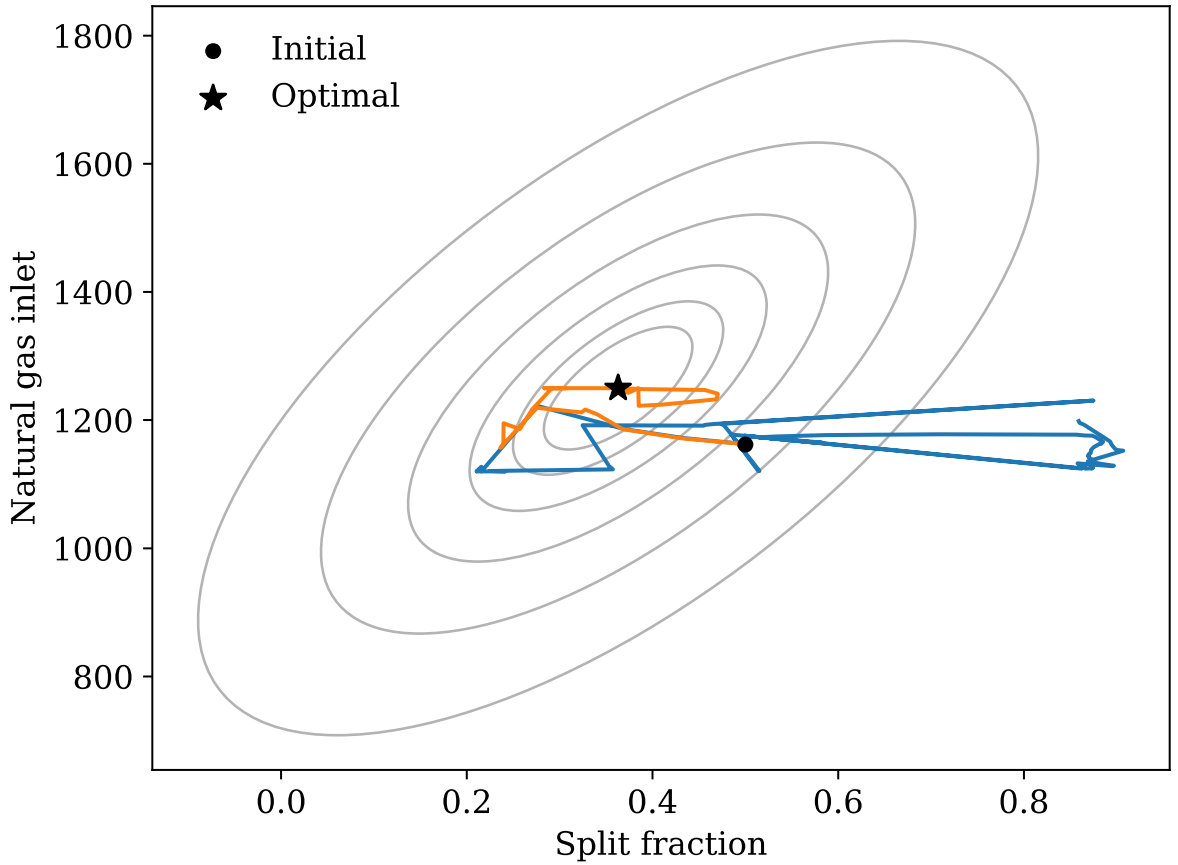
$$\mathcal{H} = \nabla_{xx}\mathcal{L} + \nabla_x g^T \Sigma_g \nabla_x g$$

$$\underbrace{\nabla_x f = \begin{bmatrix} N & B \end{bmatrix}}_{\text{Partition equality Jacobian}}$$

$$\underbrace{Z = \begin{bmatrix} I \\ -B^{-1}N \end{bmatrix}}_{\text{Null space basis}}$$

$$\underbrace{R = Z^T \mathcal{H} Z}_{\text{Reduced Hessian}}$$

It is sometimes useful to record variable values at each iteration of a solve



What can I do for PyNumero?

1. Reduced gradient or SQP method
2. Sparse, globalized Newton method
3. Direct interfaces to more solvers (e.g., Knitro)
4. Interfaces to more linear solvers (e.g., MA28, MA48, cuDSS)
5. Bilevel optimization (via ExternalGreyBoxBlock)

Questions?