CSSI Element: *libkrylov* - a Modular Open-Source Software Library for Extremely Large Eigenvalue and Linear Problems

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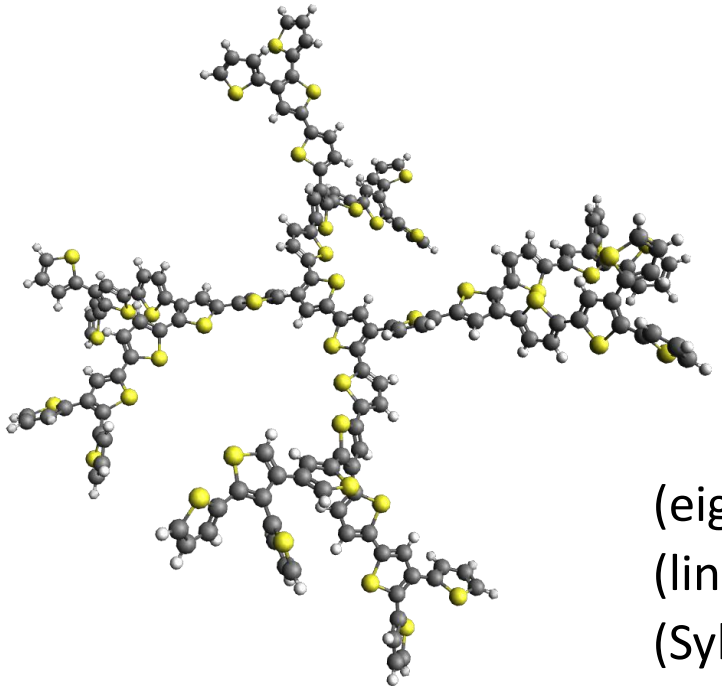
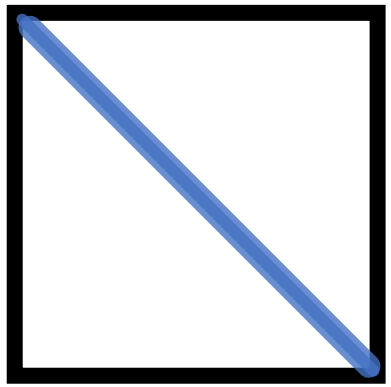
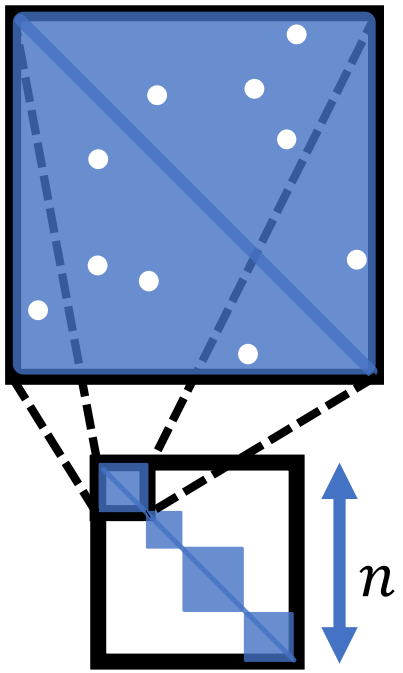
42- unit polythiophene dendrimer
n = 15782742



Sparse $\mathbf{A}$



Dense, Structured $\mathbf{A}$



Solving for

$$\mathbf{X} = \{X_1\ X_2\ \ldots X_p\},$$

(eigenvalue) $\mathbf{A}X_j = \Omega_j X_j$

(linear) $\mathbf{A}X_j = P_j$

(Sylvester) $\mathbf{A}X_j - \omega_j X_j = P_j$

Public Repository at: gitlab.com/libkrylov (3-Clause BSD)

Code Snippets

```
module user_functions
  type, extends(signatures) :: user_f
    ⋮
    integer :: input
    real, pointer :: output
    ⋮
  contains
    procedure :: deferred => mvproduct
  end type
end module user_functions
```

```
  ⋮
  use libkrylov
  use user_functions
  ⋮
  type(user_f) :: functions
  ⋮
  functions%input  = input
  functions%output => output
  ierr = 0
  call libkrylov_solver(functions,ierr)
  ⋮
```

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