Recent advances with PETSc in FreeFEM

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11th FreeFEM days

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Introduction

1. Introduction
2. Operator
3. Linear solvers
4. Eigensolvers
5. Nonlinear solvers
6. Applications

Introduction

PETSc

- Portable, Extensible Toolkit for Scientific Computation
- suite of data structures
  - `Vec` and `Mat`
  - `PC` and `KSP`
  - `SNES`, `TS`, and `Tao`

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- useful for compiling other libraries (MUMPS, *hypre*)
- `https://www.mcs.anl.gov/petsc`
- `https://gitlab.com/petsc/petsc`

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- may be compiled from the sources
- currently install the following packages
  - MUMPS
  - SuperLU
  - SuiteSparse
  - *hypre*
  - Metis
  - SCOTCH
  - TetGen
  - SLEPc
  - HPDDM

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  - MUMPS
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  - *hypre*
  - Metis
  - SCOTCH
  - TetGen
  - SLEPc
  - HPDDM
- `load "PETSc"` or `load "PETSc-complex"`
- `load "SLEPc"` or `load "SLEPc-complex"`

Operator

Mat

- same typename as in PETSc
- list of operations in the `Mat` manual pages
- same operations as with a `matrix`
    - `A * x`
    - `A' * x`
    - `A^-1 * x`
    - `A'^-1 * x`

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  - `A * x`
  - `A' * x`
  - `A^-1 * x`
  - `A'^-1 * x`
- as easy as
```
matrix a = ...
Mat A(a)
```

Block matrix

- matrix nested with submatrices or vectors
- exactly same structure with a `Mat`
- useful for multiphysics, e.g.,
```
Mat St = [[A , B],
          [B', 0]]
```
- underyling PETSc MatNest

Distributed numbering

- all this works in parallel
- FreeFEM and PETSc have their own numberings
- `changeNumbering` to go from one to the other

Linear solvers

Attaching a KSP

- for a `matrix`, `set(solver = sparsesolver)`

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  - KSP manual pages
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  - KSP manual pages
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- deprecated plugins in v4, available through PETSc

Fieldsplit

- separate preconditioners for different fields
- `fespace Vh(Pk,Pq,Pt)` ⇒ `Vh [u,v,w] = [1,2,3]`
- new KSP prefixed by `-fieldsplit_%d_`

Optional parameters

- prefixes customizable with a `string[int]`
- approximate Schur complement

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Examples for Stokes equations [Knepley 2013]

$$A = \begin{bmatrix} C & B \\ B^T & 0 \end{bmatrix} \approx \mathrm{pc}_A = \begin{bmatrix} C^{-1} & 0 \\ 0 & I \end{bmatrix}$$

-ksp_type gmres -pc_fieldsplit_type additive
-fieldsplit_velocity_pc_type lu
-fieldsplit_pressure_pc_type jacobi

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-ksp_type fgmres -pc_fieldsplit_type additive
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$$A = \begin{bmatrix} C & B \\ B^T & 0 \end{bmatrix} \approx \mathrm{pc}_A = \begin{bmatrix} \mathrm{ksp}_C & 0 \\ 0 & -\mathrm{ksp}_S \end{bmatrix}$$

-ksp_type fgmres -pc_fieldsplit_type schur
-fieldsplit_velocity_pc_type gamg
-fieldsplit_pressure_pc_type jacobi
-pc_fieldsplit_schur_factorization_type diag

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-ksp_type fgmres -pc_fieldsplit_type schur
-fieldsplit_velocity_pc_type gamg
-fieldsplit_pressure_pc_type jacobi
-pc_fieldsplit_schur_factorization_type lower

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-ksp_type gmres -fieldsplit_pressure_ksp_max_its 1
-pc_fieldsplit_type schur -fieldsplit_velocity_pc_type lu
-fieldsplit_pressure_ksp_type richardson
-pc_fieldsplit_schur_factorization_type upper

New multigrid solvers

Geometric multigrid

- FreeFEM generates a hierarchy of grids
- corresponding prolongation operators
- `PCMG` manual pages
- `diffusion-mg-3d-PETSc.edp`

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For problems in $H(\mathrm{curl})$

- AMS from *hypre* [Hiptmair and Xu 2007]
- edge to node correspondance in `mat_edgeP1`
- `maxwell-3d-PETSc.edp`

Eigensolvers

EPSSolve

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- `EigenValue` uses ARPACK
- not much versatility
- `EPSSolve(A)`, `EPSSolve(A,B)`
- `EPSSolve(func)`
- spectral transformations relies on a `KSP`
  - `EPSSolve(A, sparams = "...")`
  - `set(A, sparams = "...")`

    $\Rightarrow$ object composability
- `EPS` manual pages

Nonlinear solvers

SNESSolve

- easy-to-use interface to (quasi-)Newton methods
- solve $\mathcal{F}(u) = b$
- handle variational inequalities on u

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- easy-to-use interface to (quasi-)Newton methods
- solve $\mathcal{F}(u) = b$
- handle variational inequalities on u
- must provide two `func`s
    - to evaluate residuals stored as `K[int]`
    - to update a Jacobian stored as `Mat`
      $\Rightarrow$ object composability, `KSP` attached to the `Mat`
- `SNES` manual pages

Timesteppers and optimizers

`TSSolve` [Abhyankar et al. 2018]

- for DAE and ODE s.t. $F(t, u, \dot{u}) = G(u, t)$
- implicit, explicit, and IMEX methods
- `advection-TS-2d-PETSc.edp`
- `TS` manual pages

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- `TS` manual pages

`TaoSolve`

- similar interface to Ipopt
- `minimal-surface-Tao-2d-PETSc.edp`
- `Tao` manual pages

Applications

BEM

Contribution from P. Marchand (UOB)

- preconditioning with a FE mass matrix
- 26 GHz on 256 MPI processes, 111k unknowns
- `helmholtz-3d-surf-PETSc-complex.edp`

Preconditioning	None	M^{-1}
Solve (seconds)	122	91
# of iterations	1,649	1,271

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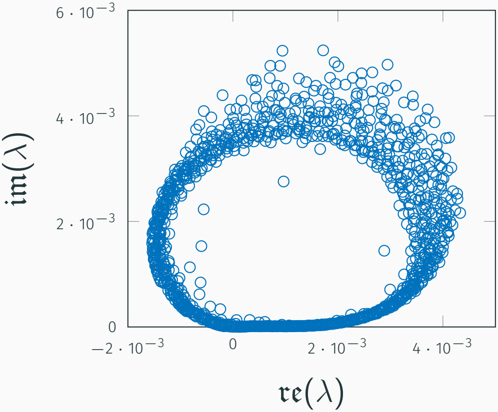

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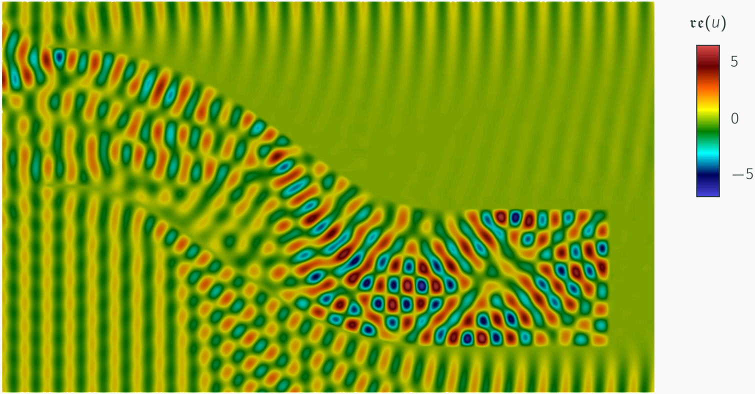
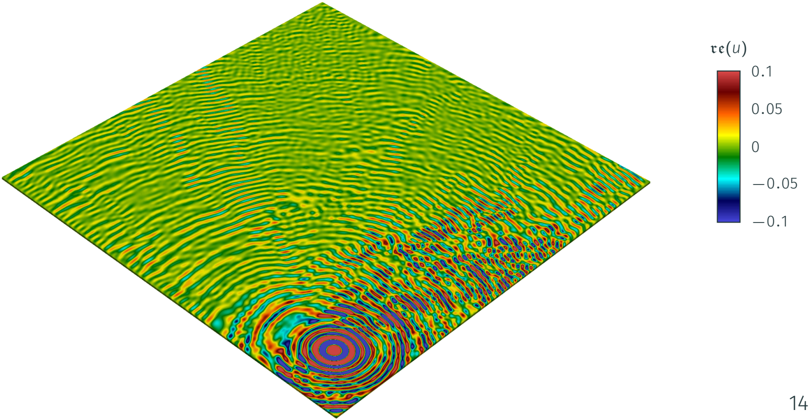


PCMG with optimized Schwarz methods

- overthrust model at 10 Hz on 512 MPI processes
- subdomains with $\approx$ 600k unknowns $\Rightarrow$ 344 seconds



Contribution from M. A. Badri (CEA) and Y. Favennec (LTEN)

Semi-discretized RTE

$$\forall m \in [\![1; N_d]\!], \left(\vec{s}_m \cdot \nabla + (\kappa + \sigma)\right) I_m = \sigma \sum_{n=1}^{N_d} \omega_n \varphi_{m,n} \cdot I_n + \kappa B$$

Radiative Transfer

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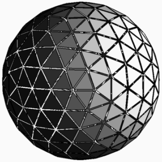
$N_d = 80$



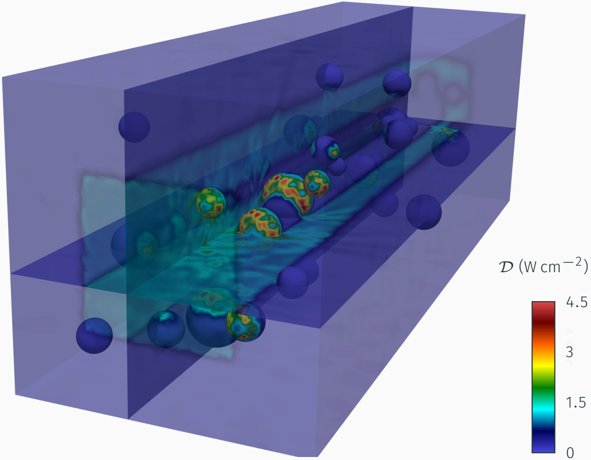
$N_d = 320$

$$\vec{s}_m = \begin{bmatrix} \sin\theta_m \cos\psi_m \\ \sin\theta_m \sin\psi_m \\ \cos\theta_m \end{bmatrix}$$

- κ (resp. σ) absorption (resp. scattering) coefficient
- φ phase scattering function
- B black body emissivity function

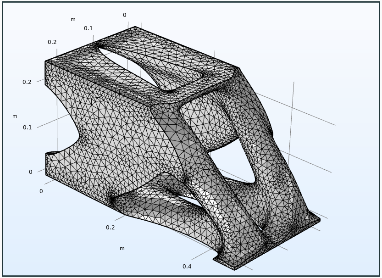
Radiative Transfer

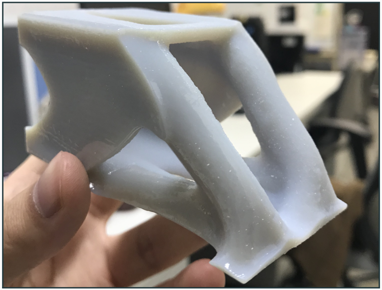
- matrix-free solver with BoomerAMG preconditioning
- 45×10^9 unknowns, 24k MPI processes
- 3.4×10^{15} nonzero entries



From design to manufacturing

Contribution from L. Hao, T. Yamada, S. Nishiwaki (Kyoto U.)





Augmented Lagrangian

grad–div stabilization [Benzi and Olshanskii 2006]

$$\begin{bmatrix} J_{uu} + \gamma J_{pu}^T W^{-1} J_{up} & J_{pu}^T \\ J_{pu} & 0 \end{bmatrix} \begin{bmatrix} u \\ p \end{bmatrix} = \begin{bmatrix} f_{u,\gamma} \\ f_p \end{bmatrix}$$

with $f_{u,\gamma} = f_u + J_{pu}^T W^{-1} f_p$

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Augmented Lagrangian preconditioning

$$P_{\mathrm{AL}} = \begin{bmatrix} J_{uu,\gamma} & 0 \\ J_{pu} & S_p \end{bmatrix}$$

with $S_p^{-1} = -\nu M_p^{-1} - \gamma W^{-1}$ [Farrell et al. 2019]

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with $f_{u,\gamma} = f_u + J_{pu}^T W^{-1} f_p$

Augmented Lagrangian preconditioning

$$P_{\mathrm{mAL}} = \begin{bmatrix} \begin{bmatrix} J_{u_x u_x,\gamma} & J_{u_x u_y,\gamma} \\ J_{u_y u_x,\gamma} & J_{u_y u_y,\gamma} \end{bmatrix} & 0 \\ J_{pu} & S_p \end{bmatrix}$$

with $S_p^{-1} = -\nu M_p^{-1} - \gamma W^{-1}$ [Farrell et al. 2019]

Augmented Lagrangian

grad–div stabilization [Benzi, Olshanskii, and Wang 2011]

$$\begin{bmatrix} J_{uu} + \gamma J_{pu}^T W^{-1} J_{up} & J_{pu}^T \\ J_{pu} & 0 \end{bmatrix} \begin{bmatrix} u \\ p \end{bmatrix} = \begin{bmatrix} f_{u,\gamma} \\ f_p \end{bmatrix}$$

with $f_{u,\gamma} = f_u + J_{pu}^T W^{-1} f_p$

Modified augmented Lagrangian preconditioning

$$P_{\mathrm{mAL}} = \begin{bmatrix} \begin{bmatrix} J_{u_x u_x,\gamma} & 0 \\ J_{u_y u_x,\gamma} & J_{u_y u_y,\gamma} \end{bmatrix} & 0 \\ J_{pu} & S_p \end{bmatrix}$$

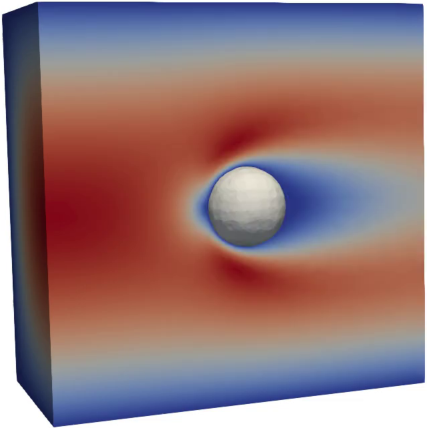
with $S_p^{-1} = -\nu M_p^{-1} - \gamma W^{-1}$ [Moulin et al. 2019]

$\Longrightarrow$ `https://github.com/prj-/moulin2019al`

Shape optimization

Contribution from F. Feppon, G. Allaire (CMAP), C. Dapogny (LJK)

- maximizing the lift of a structure



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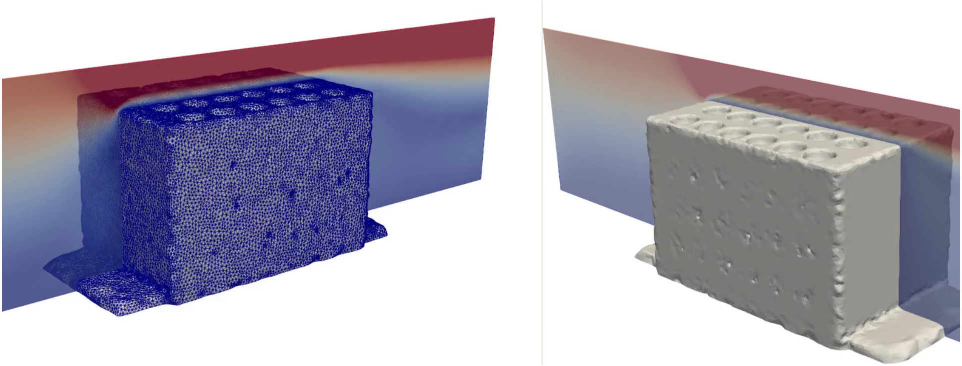
- maximizing the lift of a structure
- minimizing the compliance of a structure



Contribution from J. Moulin and O. Marquet (ONERA)

$$J = \begin{bmatrix} J_{ss} & 0 & 0 & J_{s\lambda} \\ J_{es} & J_{ee} & 0 & 0 \\ 0 & J_{qe} & J_{qq} & J_{q\lambda} \\ 0 & 0 & J_{\lambda q} & 0 \end{bmatrix} \Longrightarrow$$

```
Mat J = [[Jss,0  ,0  ,Jsl],
         [Jes,Jee,0  ,  0],
         [0  ,Jqe,Jqq,Jql],
         [0  ,0  ,Jlq,0  ]];
```

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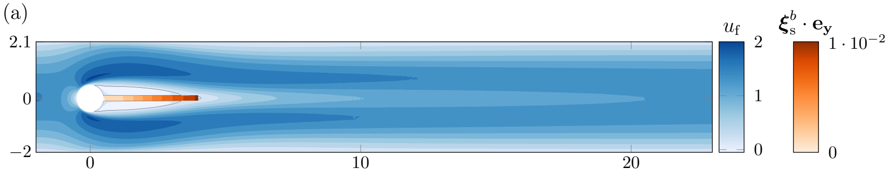
         [0  ,Jqe,Jqq,Jql],
         [0  ,0  ,Jlq,0  ]];
```

- fieldsplit for the outer PC [Deparis et al. 2016]
- `set(sparams = "...")` for the diagonal blocks
- nested fieldsplit for `Jqq`

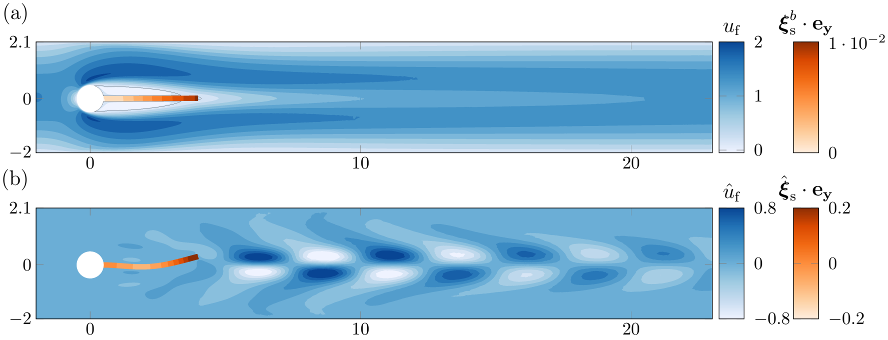
Contribution from J. Moulin and O. Marquet (ONERA)



Baseflow

[Turek and Hron 2006]

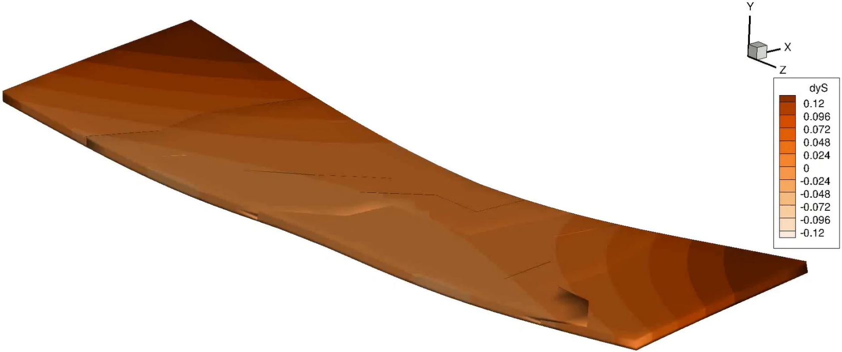
Contribution from J. Moulin and O. Marquet (ONERA)



Baseflow and leading eigenmode [Turek and Hron 2006]

Fluid–structure interaction

Contribution from J. Moulin and O. Marquet (ONERA)



Final words

- multiphysics solvers with PETSc and FreeFEM
  - high level of abstraction of FreeFEM
  - versatility of PETSc
- composability of solvers
- ongoing developments are user-driven
- `jolivet.perso.enseeiht.fr/FreeFem-tutorial`
- automatic differentiation?

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Thank you!

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