Simulation Components in PETSc

Matt Knepley, Mark Adams, Joseph Pusztay, Danny Finn

Computer Science and Engineering
University at Buffalo

NumKin 2023
Max Planck Institut für Plasmaphysik, Garching, DE
Nov 7, 2023

University at Buffalo
Center for Hybrid Rocket
Exascale Simulation Technology

Never believe anything

until you run it.

Outline

Unstructured and Semistructured grids

Discretizatons

Solvers

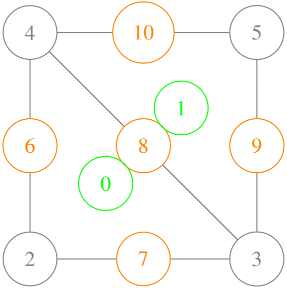
Examples

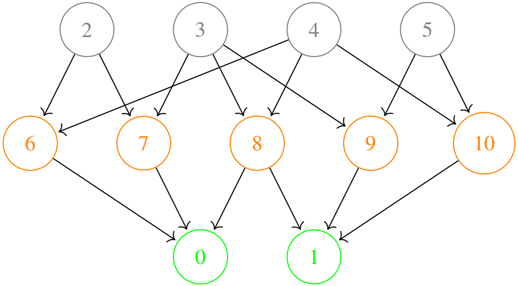
Unstructured Meshes

PETSc DMPlex

PETSc supports unstructured and structured adaptive meshes using the DMPlex object.

- Dimension independent



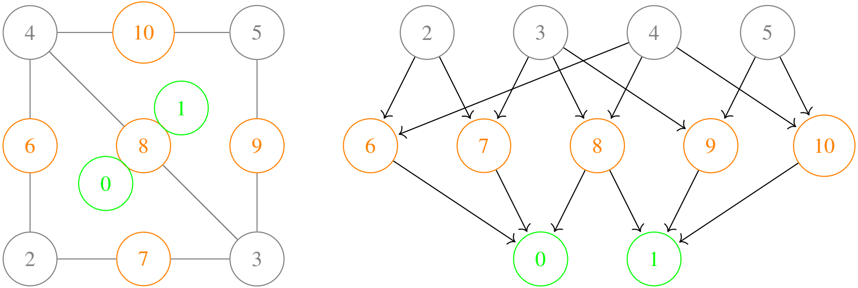


Unstructured Meshes

PETSc DMPlex

PETSc supports unstructured and structured adaptive meshes using the DMPlex object.

- Dimension independent
- Supports hybrid meshes

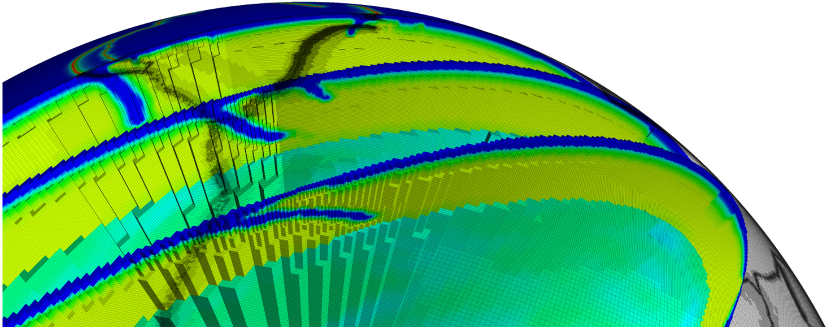


Unstructured Meshes

PETSc DMPlex

PETSc supports unstructured and structured adaptive meshes using the DMPlex object.

- Dimension independent
- Supports hybrid meshes
- Structured adaptive through p4est (Isaac and Knepley 2017)



Unstructured Meshes

PETSc DMPlex

PETSc supports unstructured and structured adaptive meshes using the DMPlex object.

- Dimension independent
- Supports hybrid meshes
- Structured adaptive through p4est (Isaac and Knepley 2017)

Plex supports many common operations, in parallel,

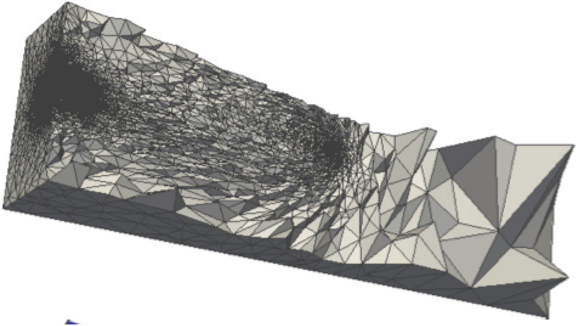
- refinement
- extrusion
- cell conversion
- edge/face creation

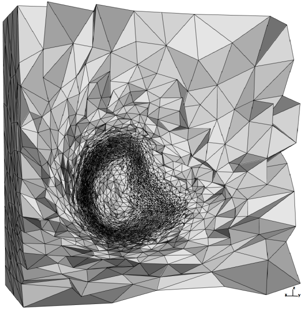
Unstructured Meshes

PETSc DMPlex

PETSc supports unstructured and structured adaptive meshes using the DMPlex object.

- Dimension independent
- Supports hybrid meshes
- AMR: (Barral et al. 2016), (Wallwork et al. 2022)





Unstructured Meshes

PETSc DMPlex

PETSc supports unstructured and structured adaptive meshes using the DMPlex object.

- Dimension independent
- Supports hybrid meshes
- AMR: (Barral et al. 2016), (Wallwork et al. 2022)

Plex publications:

(Knepley and Karpeev 2009)

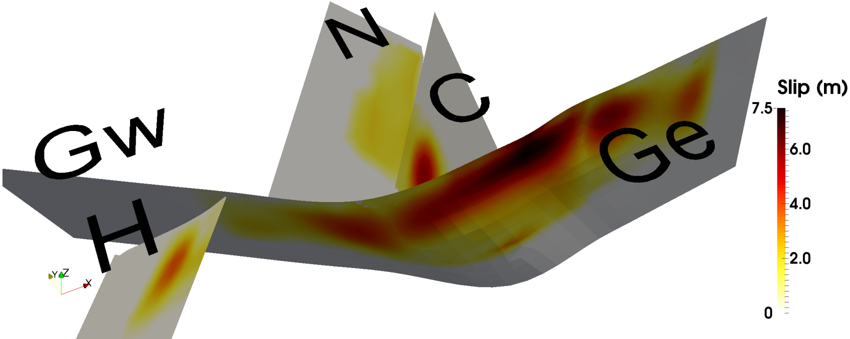
(Lange et al. 2016)

(Knepley, Lange, and Gorman 2017)

DMPlex Applications

Plex has been used in many large-scale applications:

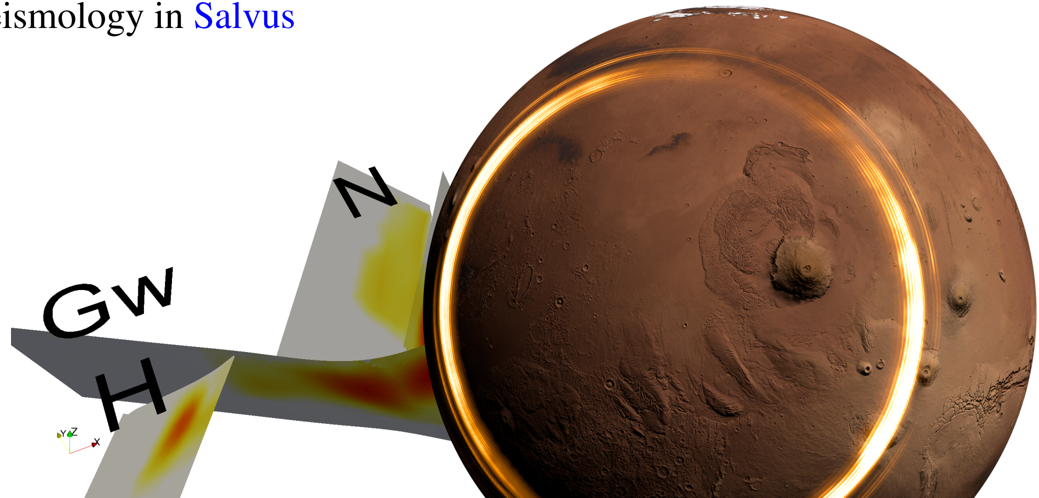
- Crustal deformation in PyLith



DMPlex Applications

Plex has been used in many large-scale applications:

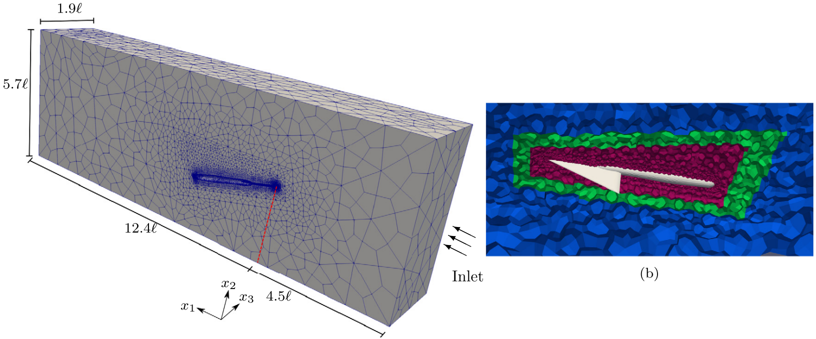
- Crustal deformation in PyLith
- Seismology in Salvus



DMPlex Applications

Plex has been used in many large-scale applications:

- Crustal deformation in PyLith
- Seismology in Salvus
- Compressible Navier-Stokes flow in SSDC



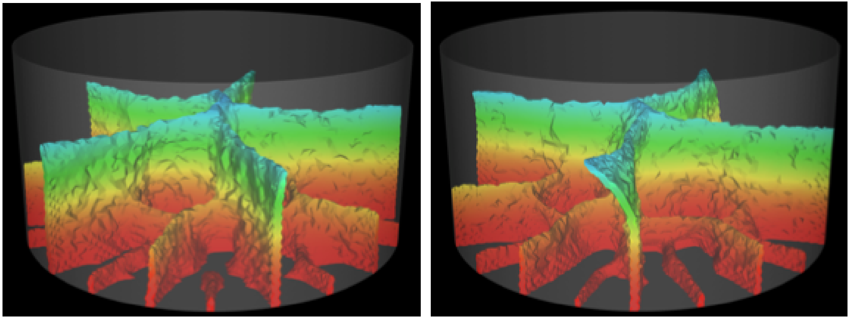
(a)

(b)

DMPlex Applications

Plex has been used in many large-scale applications:

- Crustal deformation in PyLith
- Seismology in Salvus
- Compressible Navier-Stokes flow in SSDC
- Fracture mechanics in MEF90



Example: Toroidal Mesh

Example: Toroidal Mesh

Phase 1: Create one poloidal plane and distribute

```
-phase1_dm_plex_filename /path/to/plane.mesh
-phase1_dm_plex_simplex 0 -phase1_dm_refine_pre 1
```

Example: Toroidal Mesh

Phase 1: Create one poloidal plane and distribute

```
-phase1_dm_plex_filename /path/to/plane.mesh
-phase1_dm_plex_simplex 0 -phase1_dm_refine_pre 1
```

Phase 2: Refine in parallel

```
-phase2_dm_refine 2
```

Example: Toroidal Mesh

Phase 1: Create one poloidal plane and distribute

```
-phase1_dm_plex_filename /path/to/plane.mesh
-phase1_dm_plex_simplex 0 -phase1_dm_refine_pre 1
```

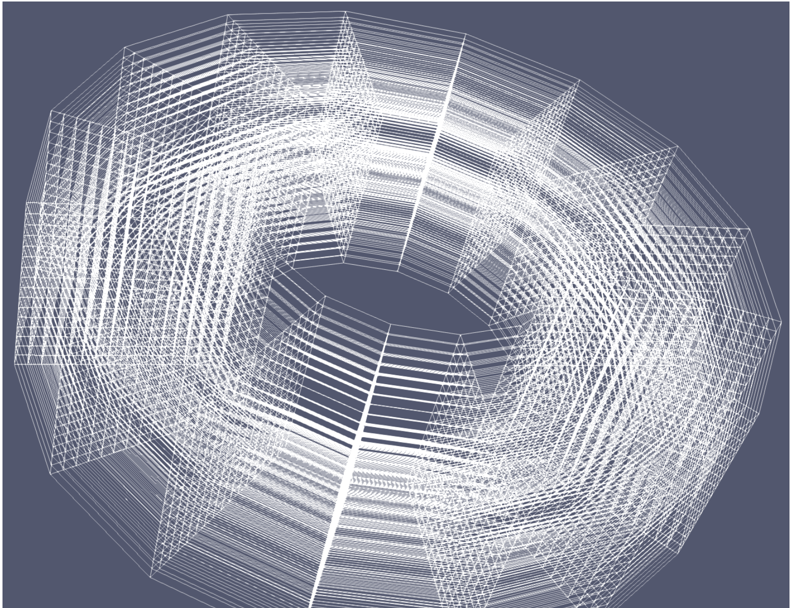
Phase 2: Refine in parallel

```
-phase2_dm_refine 2
```

Phase 3: Extrude periodically

```
-phase3_dm_plex_transform_type extrude -phase3_dm_extrude 16
-phase3_dm_plex_transform_extrude_thickness 1
-phase3_dm_plex_transform_extrude_use_tensor false
-phase3_dm_plex_transform_extrude_periodic
-phase3_dm_extrude_levels 2
```

Example: Toroidal Mesh



Outline

Unstructured and Semistructured grids

Discretizatons

Solvers

Examples

Continuum Discretizations

PetscFE

Build spaces using

- $\mathcal{P}$
- $\mathcal{P}^-$
- direct sum
- direct product

Pointwise dual spaces are built topologically

Support L_2, H^1, $H(\text{div})$, $H(\text{curl})$ spaces

Raviart-Thomas on a Quadrilateral

```
-petscspace_type sum
-petscspace_variables 2
-petscspace_components 2
-petscspace_sum_spaces 2
-petscspace_sum_concatenate true
```

Raviart-Thomas on a Quadrilateral

```
-petscspace_type sum
-petscspace_variables 2
-petscspace_components 2
-petscspace_sum_spaces 2
-petscspace_sum_concatenate true
```

```
-sumcomp_0_petscspace_variables 2
-sumcomp_0_petscspace_type tensor
-sumcomp_0_petscspace_tensor_spaces 2
-sumcomp_0_petscspace_tensor_uniform false
-sumcomp_0_tensorcomp_0_petscspace_degree <k>
-sumcomp_0_tensorcomp_1_petscspace_degree <k-1>
```

Raviart-Thomas on a Quadrilateral

```
-sumcomp_1_petscspace_variables 2
-sumcomp_1_petscspace_type tensor
-sumcomp_1_petscspace_tensor_spaces 2
-sumcomp_1_petscspace_tensor_uniform false
-sumcomp_1_tensorcomp_0_petscspace_degree <k-1>
-sumcomp_1_tensorcomp_1_petscspace_degree <k>
```

Raviart-Thomas on a Quadrilateral

```
-sumcomp_1_petscspace_variables 2
-sumcomp_1_petscspace_type tensor
-sumcomp_1_petscspace_tensor_spaces 2
-sumcomp_1_petscspace_tensor_uniform false
-sumcomp_1_tensorcomp_0_petscspace_degree <k-1>
-sumcomp_1_tensorcomp_1_petscspace_degree <k>

-petscdualspace_form_degree -1
-petscdualspace_order <k>
-petscdualspace_lagrange_trimmed true
```

Continuum Discretizations

PetscFV

Constant and linear reconstruction

Pointwise Riemann solvers

Library of limiters

Interoperates with PetscFE

Handles hanging nodes

Particle Discretizations

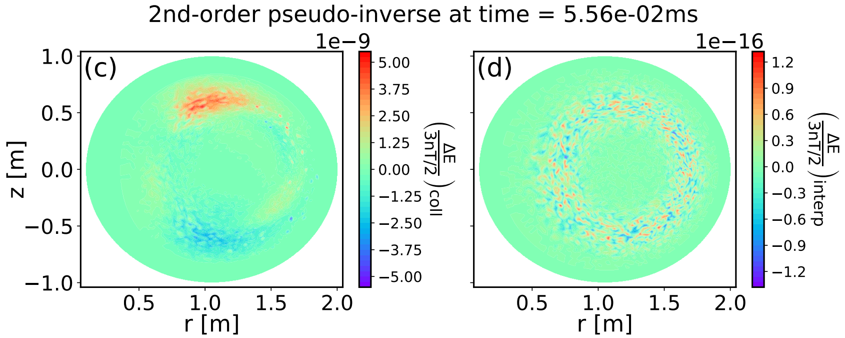
PETSc DMSwarm

PETSc supports particle discretizations using the DMSwarm object.

- Arbitrary particle data
- Scalable particle push
- Scalable point location for unstructured meshes
- Conservative projection from/onto FEM bases

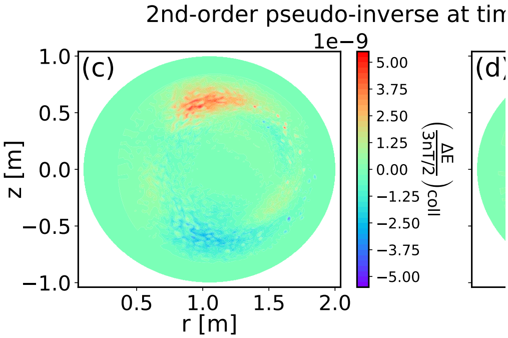
Swarm has been used in a few of large-scale applications:

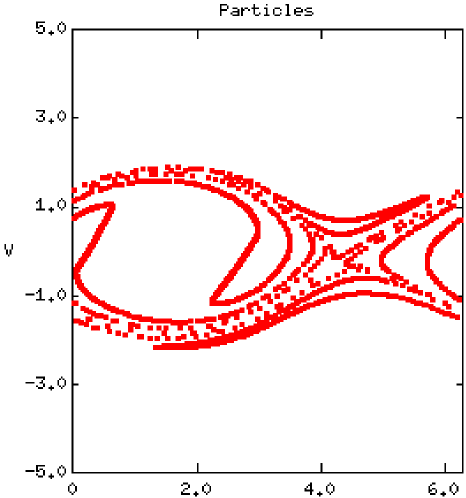
- Plasma kinetics in XGC1



Swarm has been used in a few of large-scale applications:

- Plasma kinetics in XGC1



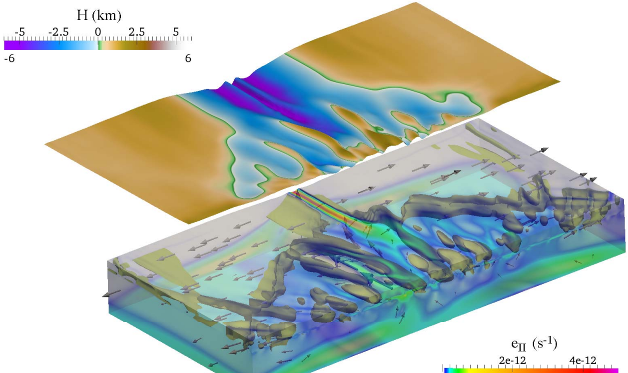


Particle Discretizations

Swarm Applications

Swarm has been used in a few of large-scale applications:

- Plasma kinetics in XGC1
- Geodynamics in ptatin3d



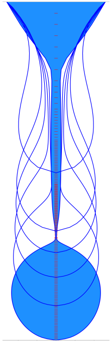
Particle Discretizations

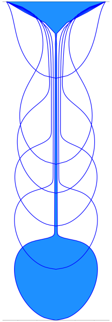
Swarm Applications

Swarm has been used in a few of large-scale applications:

- Plasma kinetics in XGC1
- Geodynamics in ptatin3d
- Plan to use for droplets in Ablate

Gravity Droplet





Shear Droplet

Outline

Unstructured and Semistructured grids

Discretizatons

Solvers

Examples

Linear and Nonlinear

- Many, many solvers and preconditioners
- Focus on optimal, multilevel solvers
- Patch multgrid
- Nonlinear preconditioners

Solving the Discrete Gradients System

Line-Search Newton (`-snes_type newtonls`)

Solving the Discrete Gradients System

Line-Search Newton (`-snes_type newtonls`)

Green function for Laplace is dense

Solving the Discrete Gradients System

Line-Search Newton (`-snes_type newtonls`)

Act with FD residual, include block-diagonal in pmat

(`-snes_mf_operator -pc_type lu -pc_factor_mat_solver_type mumps`)

Solving the Discrete Gradients System

Line-Search Newton (`-snes_type newtonls`)

- Act with FD residual, include block-diagonal in pmat (`-snes_mf_operator -pc_type lu -pc_factor_mat_solver_type mumps`)
- DG Gonzalez term has global coupling

Solving the Discrete Gradients System

Line-Search Newton (`-snes_type newtonls`)

Act with FD residual, include block-diagonal in pmat
(`-snes_mf_operator -pc_type lu -pc_factor_mat_solver_type mumps`)

Represent preconditioning matrix as $A + UCV^T$
(use `MatLRC` type)

Solving the Discrete Gradients System

Preconditioning matrix might be far from true matrix

Line-Search Newton (`-snes_type newtonls`)

- Act with FD residual, include block-diagonal in pmat (`-snes_mf_operator -pc_type lu -pc_factor_mat_solver_type mumps`)
- Represent preconditioning matrix as $A + UCV^T$ (use `MatLRC` type)

Solving the Discrete Gradients System

- Precondition Newton using Richardson (`-snes_npc_type nrichardson`)
- Line-Search Newton (`-snes_type newtonls`)
  - Act with FD residual, include block-diagonal in pmat (`-snes_mf_operator -pc_type lu -pc_factor_mat_solver_type mumps`)
  - Represent preconditioning matrix as $A + UCV^T$ (use `MatLRC` type)

Timestepping

- Explicit, Implicit, and IMEX formulations
- Symplectic methods
- Index 1 and 2 Differential-Algebraic Equations (DAE)
- Adaptivity and error control
- Discrete Adjoints and Sensitivity Analysis
- Handles events and discontinuities

Optimization

- Minimization
  - Unconstrained
  - Bound-Constrained Optimization
  - Generally Constrained Solvers
- Nonlinear Least-Squares
  - Bound-constrained Regularized Gauss-Newton
  - Derivative-Free
- Complementarity
- PDE-constrained Optimization

Eigensolves

- Linear Eigenvalue Problem
- Singular Value Decomposition
- Polynomial Eigenvalue Problem
- Nonlinear Eigenvalue Problem
- Matrix Function
- Linear Matrix Equation

Outline

Unstructured and Semistructured grids

Discretizatons

Solvers

Examples

- Conservative Projection

Outline

Examples

Conservative Projection

Integrating into PETSc,

we get support and

long term maintenance.

Using linear algebra interfaces,

we get portability

and optimization.

Abstracting operations,

enables composition and

new algorithmic choices.

By designing library interfaces,

we can embed PIC in

more complex simulations.

As an example, let us derive:

Conservative projection operators

between Particle and FEM spaces.

$$\int f = \int f$$

where

$$f \in \mathcal{F} \qquad f \in \mathcal{P}$$

$$\int \vec{x} f = \int \vec{x} f$$

where

$$f \in \mathcal{F} \qquad f \in \mathcal{P}$$

$$\int x^2 f = \int x^2 f$$

where

$$f \in \mathcal{F} \qquad f \in \mathcal{P}$$

Linear Algebra

$$\int \phi_i f = \int \phi_i f \qquad \forall \phi_i \in \mathcal{F}$$

where

$$f \in \mathcal{F} \qquad f \in \mathcal{P}$$

Linear Algebra

$$\int \phi_i \sum_j c_j \phi_j = \int \phi_i \sum_p w_p \, \delta(\vec{x} - \vec{x}_p)$$

Linear Algebra

$$\int \phi_i \sum_j c_j \phi_j = \int \phi_i \sum_p w_p \delta(\vec{x} - \vec{x}_p)$$

which in linear algebra terms is

$$Mc = Vw$$

Linear Algebra

$$\boldsymbol{M}_{ij} = \int \phi_i \phi_j$$

$$\boldsymbol{V}_{ip} = \int \phi_i \, \delta(\vec{x} - \vec{x}_p)$$

Linear Algebra

FEM coef. from particle weights:

$$c = M^{-1} V w$$

FEM rhs from particle weights:

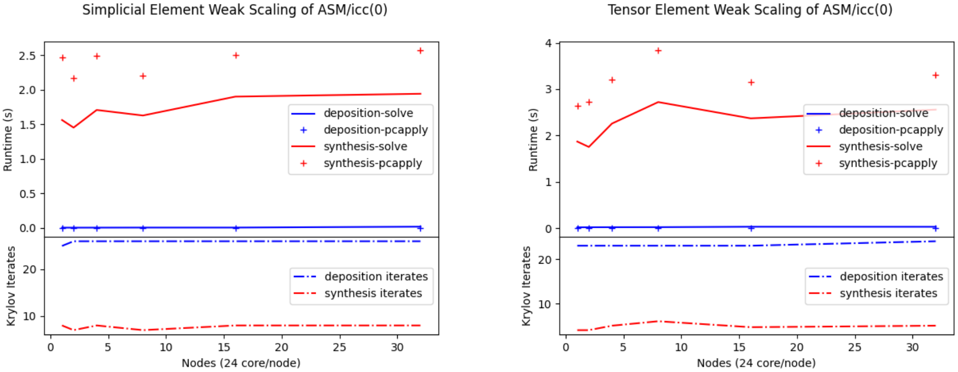
$$\int \phi_i f = M c = V w$$

Particle weights from FEM field:

$$w = V^{+} M c$$

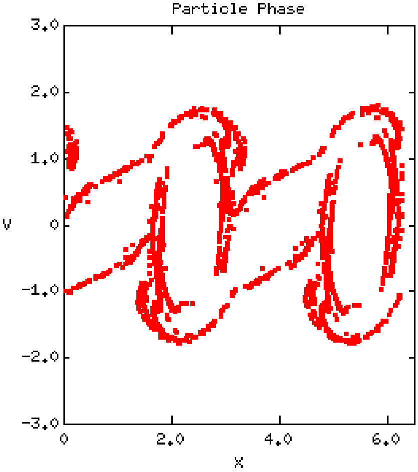
Pseudo-inverse is block-diagonal
with a DG basis.

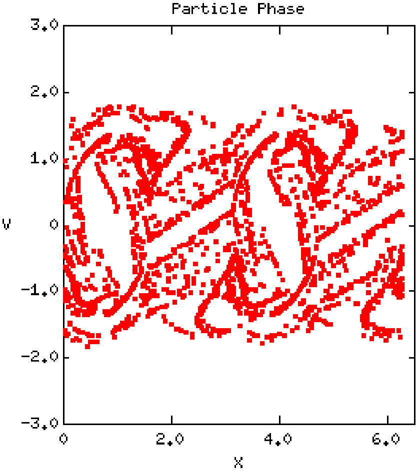
Scaling



Simplicial Element Weak Scaling of ASM/icc(0)
Runtime (s)
Krylov Iterates
Nodes (24 core/node)
deposition-solve
deposition-pcapply
synthesis-solve
synthesis-pcapply
deposition iterates
synthesis iterates
Tensor Element Weak Scaling of ASM/icc(0)
Runtime (s)
Krylov Iterates
Nodes (24 core/node)
deposition-solve
deposition-pcapply
synthesis-solve
synthesis-pcapply
deposition iterates
synthesis iterates

PETSc TS tutorials/hamiltonian/ex2





Embedding

All tests may be reproduced:

- Install PETSc www.mcs.anl.gov/petsc

```
cd $PETSC_DIR
make -f ./gmakefile test
   search="ts_tutorials_hamiltonian-ex2*"

cd src/ts/tutorials/hamiltonian
make ex2
```

- Test options at the end of the source file

My Focus

Solvers

My Focus

Efficient,

Solvers

My Focus

Efficient,

Scalable,

Solvers

My Focus

Efficient,

Scalable,

Solvers

for Multiscale,

My Focus

Efficient,

Scalable,

Solvers

for Multiscale,

Multiphysics

Problems

My Focus

Ingredients for GEMPIC:

- Symplectic integrator
- Conservative Projection
- Continuous E-field
- Entropic Integrator
- Collision Operator

Abstraction

We can dynamically select:

- FEM discretization
- Particle layout
- Background mesh
- Poisson solver
- Projection solver
- Time integrators

References I

- Isaac, Tobin and Matthew G. Knepley (2017). "Support for Non-conformal Meshes in PETSc's DMPlex Interface". In: ArXiv e-prints. http://arxiv.org/abs/1508.02470. eprint: 1508.02470.
- Knepley, Matthew G. and Dmitry A. Karpeev (2009). "Mesh Algorithms for PDE with Sieve I: Mesh Distribution". In: Scientific Programming 17.3. http://arxiv.org/abs/0908.4427, pp. 215–230. DOI: 10.3233/SPR-2009-0249. URL: http://arxiv.org/abs/0908.4427.
- Lange, Michael, Lawrence Mitchell, Matthew G. Knepley, and Gerard J. Gorman (2016). "Efficient mesh management in Firedrake using PETSc-DMPlex". In: SIAM Journal on Scientific Computing 38.5, S143–S155. DOI: 10.1137/15M1026092. eprint: http://arxiv.org/abs/1506.07749.
- Knepley, Matthew G., Michael Lange, and Gerard J. Gorman (2017). "Unstructured Overlapping Mesh Distribution in Parallel". In: ArXiv e-prints. http://arxiv.org/abs/1506.06194. eprint: 1506.06194.
- Hapla, Vaclav, Matthew G. Knepley, Michael Afanasiev, Christian Boehm, Martin van Driel, Lion Krischer, and Andreas Fichtner (2021). "Fully Parallel Mesh I/O using PETSc DMPlex with an Application to Waveform Modeling". In: SIAM Journal on Scientific Computing 43.2, pp. C127–C153. DOI: 10.1137/20M1332748. eprint: http://arxiv.org/abs/2004.08729.
- Barral, Nicolas, Matthew G. Knepley, Michael Lange, Matthew D. Piggott, and Gerard J. Gorman (Sept. 2016). "Anisotropic mesh adaptation in Firedrake with PETSc DMPlex". In: 25th International Meshing Roundtable. Ed. by Steve Owen and Hang Si. Washington, DC, pp. 1–5. URL: http://imr.sandia.gov/papers/imr25/2026_imr25RN_Barral.pdf.
- Wallwork, Joseph G., Matthew G. Knepley, Nicolas Barral, and Matthew D. Piggott (Jan. 2022). "Parallel Metric-Based Mesh Adaptation in PETSc using ParMmg". In: SIAM International Meshing Roundtable Workshop 2022. Ed. by Trevor Robinson. Seattle, WA, pp. 1–5. URL: http://imr.sandia.gov/papers/imr31/2026_imr31RJ_Wallwork.pdf.