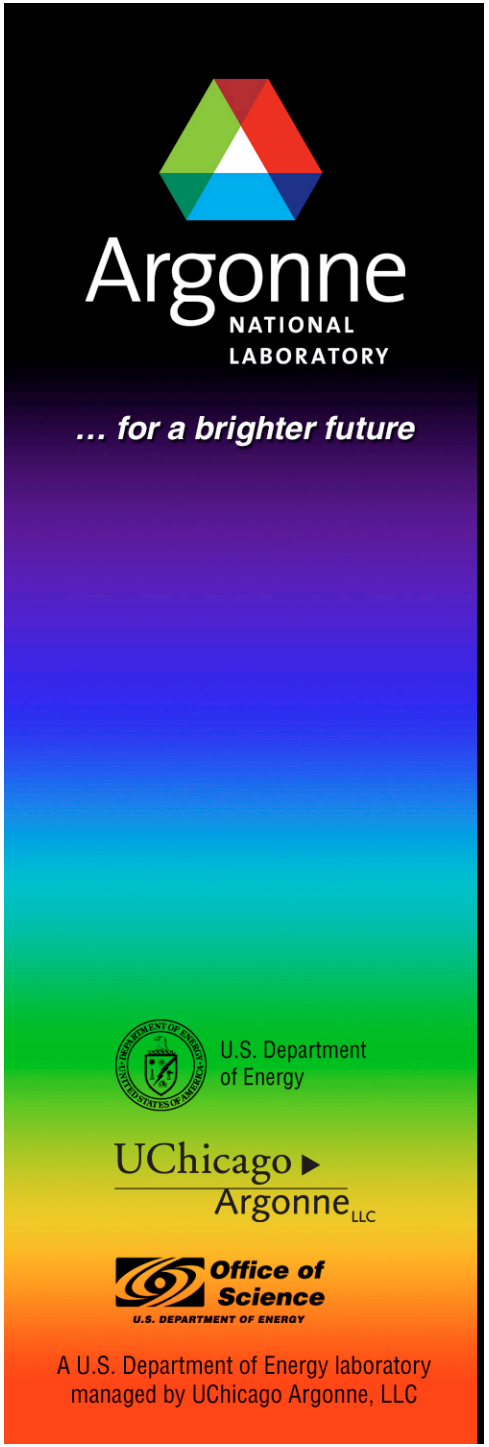


I. Portable, Extensible Toolkit for Scientific Computation

Boyana Norris

(representing the PETSc team)

Mathematics and Computer Science Division

Argonne National Laboratory, USA

March, 2009

What is PETSc?

- A freely available and supported research code
- Download from http://www.mcs.anl.gov/petsc
- Hyperlinked manual, examples, and manual pages for all routines
- Hundreds of tutorial-style examples, many are real applications
- Support via email: petsc-maint@mcs.anl.gov
- Usable from C, C++, Fortran 77/90, and Python

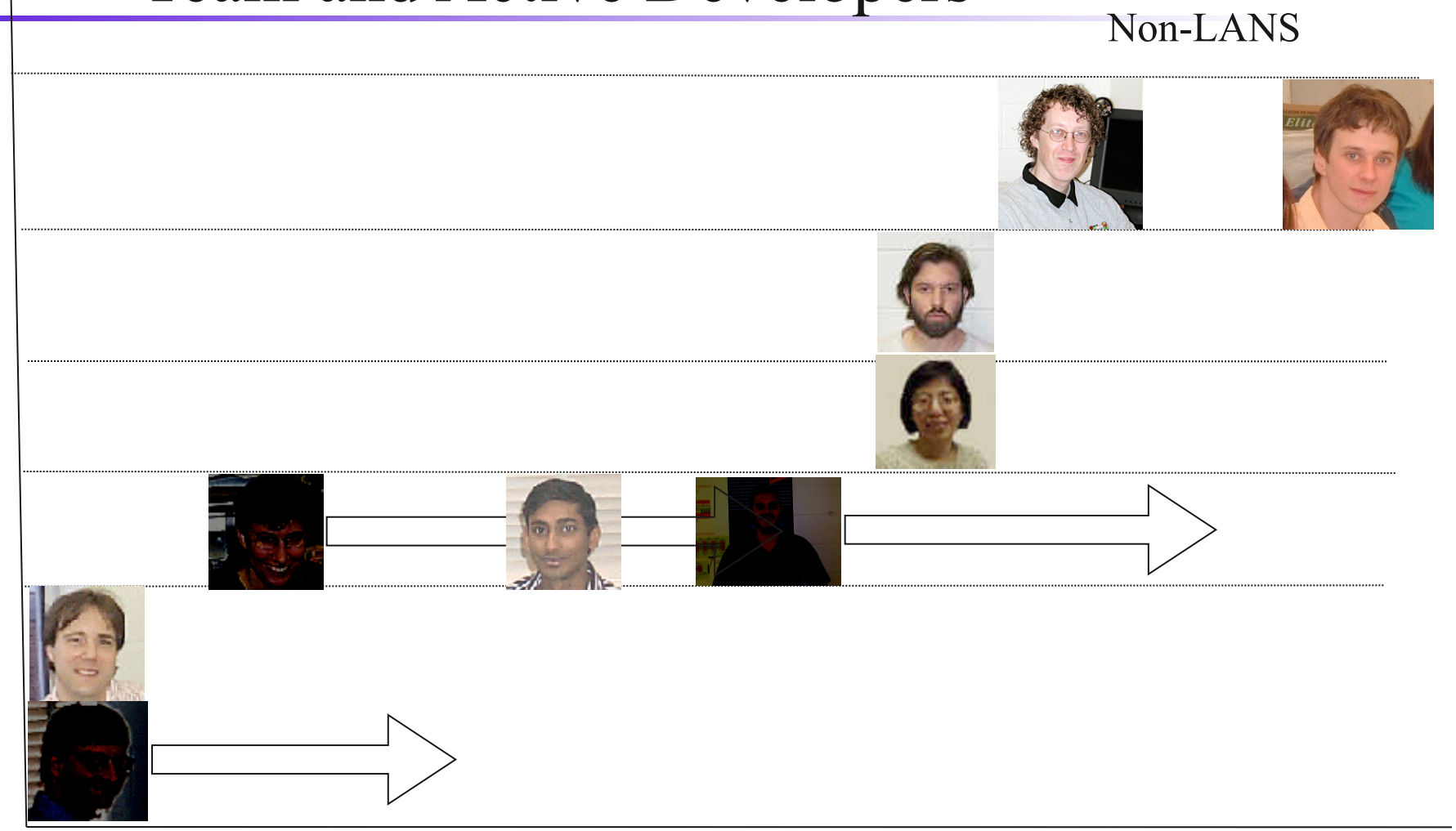
What is PETSc?

- Portable to any parallel system supporting MPI, including:
  - Tightly coupled systems
    - *Blue Gene/P, Cray XT4, Cray T3E, SGI Origin, IBM SP, HP 9000, Sub Enterprise*
  - Loosely coupled systems, such as networks of workstations
    - *Compaq,HP, IBM, SGI, Sun, PCs running Linux or Windows, Mac OS X*

- PETSc History
  - Begun September 1991
  - Over 20,000 downloads since 1995 (version 2), currently 300 per month

- PETSc Funding and Support
  - Department of Energy
    - *SciDAC, MICS Program, INL Reactor Program*
  - National Science Foundation
    - *CIG, CISE, Multidisciplinary Challenge Program*

Team and Active Developers



How did PETSc Originate?

PETSc was developed as a Platform for Experimentation.

We want to experiment with different

- Models
- Discretizations
- Solvers
- Algorithms (which blur these boundaries)

Successfully Transitioned from Basic Research to Common Community Tool

- Applications of PETSc
  - Nano-simulations (20)
  - Biology/Medical(28)
  - Cardiology
  - Imaging and Surgery
  - Fusion (10)
  - Geosciences (20)
  - Environmental/Subsurface Flow (26)
  - Computational Fluid Dynamics (49)
  - Wave propagation and the Helmholz equation (12)
  - Optimization (7)
  - Other Application Areas (68)
  - Software packages that use or interface to PETSc (30)
  - Software engineering (30)
  - Algorithm analysis and design (48)

Who Uses PETSc?

- Computational Scientists
  - PyLith (TECTON), Underworld, Columbia group
- Algorithm Developers
  - Iterative methods and Preconditioning researchers
- Package Developers
  - SIPs, SLEPc, TAO, MagPar, StGermain, Dealll

The Role of PETSc

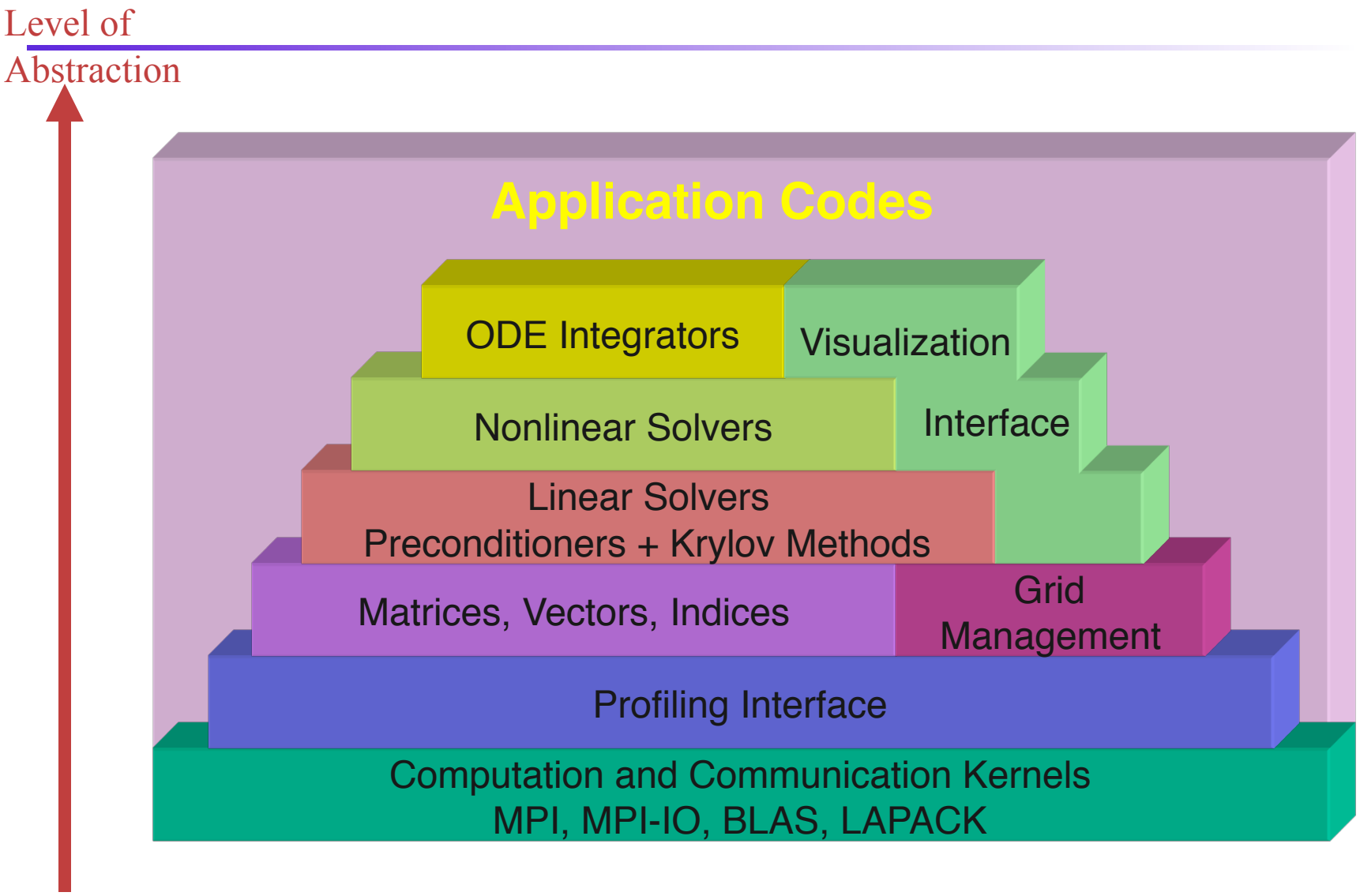
Developing parallel, nontrivial PDE solvers that deliver high performance is still difficult and requires months (or even years) of concentrated effort.

PETSc is a tool that can ease these difficulties and reduce the development time, but it is not a black-box PDE solver, nor a silver bullet.

Features

- Many (parallel) vector/array operations
- Numerous (parallel) matrix formats and operations
- Numerous linear solvers
- Nonlinear solvers
- Limited ODE integrators
- Limited parallel grid/data management
- Common interface for most DOE solver software

Structure of PETSc



Interfaced Packages

- LU (Sequential)
  - SuperLU (Demmel and Li, LBNL), ESSL (IBM), Matlab, LUSOL (from MINOS - Michael Saunders, Stanford), LAPACK, PLAPACK (van de Geijn, UT Austin), UMFPACK (Timothy A. Davis)
- Parallel LU
  - SuperLU_DIST (Demmel and Li, LBNL)
  - SPOOLES (Ashcroft, Boeing, funded by ARPA)
  - MUMPS (European)
  - PLAPACK (van de Geijn, UT Austin)
- Parallel Cholesky
  - DSCPACK (Raghavan, Penn. State)
  - SPOOLES (Ashcroft, Boeing, funded by ARPA)
  - PLAPACK (van de Geijn, UT Austin)

Interfaced Packages

- XYTlib – parallel direct solver (Fischer and Tufo, ANL)
- SPAI – Sparse approximate inverse (parallel)
  - Parasails (Chow, part of Hypre, LLNL)
  - SPAI 3.0 (Grote/Barnard)
- Algebraic multigrid
  - Parallel BoomerAMG (part of Hypre, LLNL)
  - ML (part of Trilinos, SNL)
- Parallel ICC(0) – BlockSolve95 (Jones and Plassman, ANL)
- Parallel ILU
  - BlockSolve95 (Jones and Plassman, ANL)
  - PILUT (part of Hypre, LLNL)
  - EUCLID (Hysom – also part of Hypre, ODU/LLNL)
- Sequential ILUDT (SPARSEKIT2- Y. Saad, U of MN)

Interfaced Packages

- Parititioning
  - Parmetis
  - Chaco
  - Jostle
  - Party
  - Scotch
- ODE integrators
  - Sundials (LLNL)
- Eigenvalue solvers
  - BLOPEX (developed by Andrew Knyazev)
- FFTW
- SPRN

Child Packages of PETSc

- SIPs - Shift-and-Invert Parallel Spectral Transformations
- SLEPc - scalable eigenvalue/eigenvector solver packages.
- TAO - scalable optimization algorithms
- veltisto ("optimum")- for problems with constraints which are time-independent PDEs.

- All have PETSc's style of programming

What Can We Handle?

- PETSc has run problem with 500 million unknowns
  - http://www.scconference.org/sc2004/schedule/pdfs/pap111.pdf
- PETSc has run on over 6,000 processors efficiently
  - ftp://info.mcs.anl.gov/pub/tech_reports/reports/P776.ps.Z
- PETSc applications have run at 2 Teraflops
  - LANL PFLOTRAN code
- PETSc also runs on your laptop
- Only a handful of our users ever go over 64 processors

Example 1:

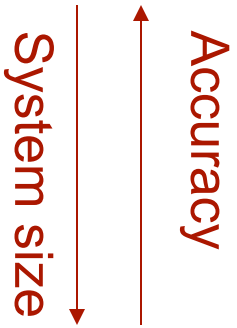
Modeling of Nanostructured Materials

- **Goal:** Characterisation/prediction of various nanoscale properties
- **Approach:** Determination and analysis of most stable atomic structure
  → Minimisation of many-particle interaction energy

$$E_{\text{tot}}(\{\vec{R}_{\text{at}}\}) = \underbrace{E_{\text{el}}(\{\vec{r}_{\text{el}}\};\{\vec{R}_{\text{at}}\})}_{\textit{hard}} + \underbrace{E_{\text{nuc}}(\{\vec{R}_{\text{at}}\})}_{\textit{“easy”}}$$

- **Methods:**

1. molecular orbital theory (Schrodinger equation)
2. density functional theory (DFT)
* 3. tight-binding (TB, **DFTB**); semi-empirical
4. classical potentials (Lennard-Jones, Brenner, . . .)



Matrices are

- large: ultimate goal
  50,000 atoms with electronic structure
  ~ N=200,000
- sparse:
  non-zero density -> 0 as N increases
- dense solutions are requested:
  60% eigenvalues and eigenvectors

Dense solutions of large sparse problems!

DFTB-eigenvalue problem is distinguished by

- (A, B) is large and sparse
  Iterative method

- A large number of eigensolutions (60%) are requested
  Iterative method + multiple shift-and-invert

- The spectrum has
  - poor average eigenvalue separation O(1/N),
  - cluster with hundreds of tightly packed eigenvalues
  - gap >> O(1/N)
  Iterative method + multiple shift-and-invert + robusness

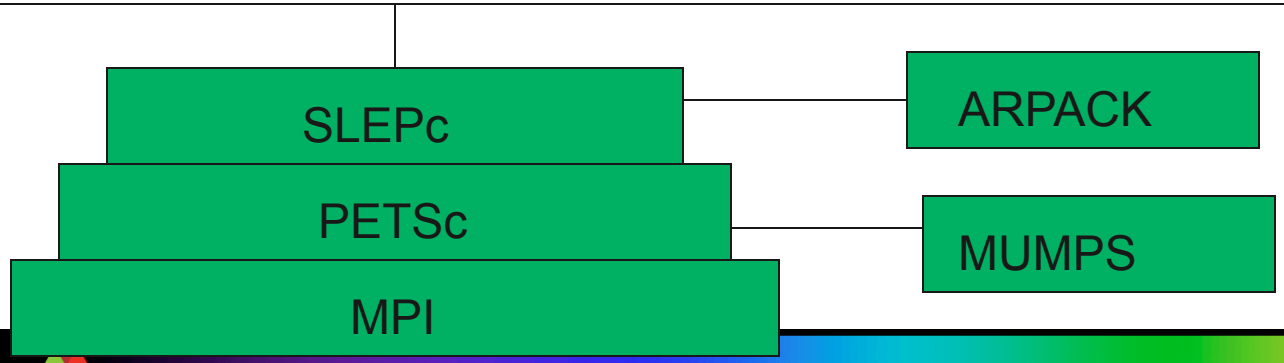
- The matrix factorization of $(A-\sigma B)=LDL^T$:
  not-very-sparse(7%) <= nonzero density <= dense(50%)
  Iterative method + multiple shift-and-invert + robusness + efficiency

- $Ax=\lambda Bx$ is solved many times (possibly 1000's)
  Iterative method + multiple shift-and-invert + robusness + efficiency
  + initial approximation of eigensolutions

Software Structure

Shift-and-**I**nvert **P**arallel Spectral Transform**s** (**SIPs**)

- Select shifts
- Bookkeep and validate eigensolutions
- Balance parallel jobs
- Ensure global orthogonality of eigenvectors
- Manage matrix storage

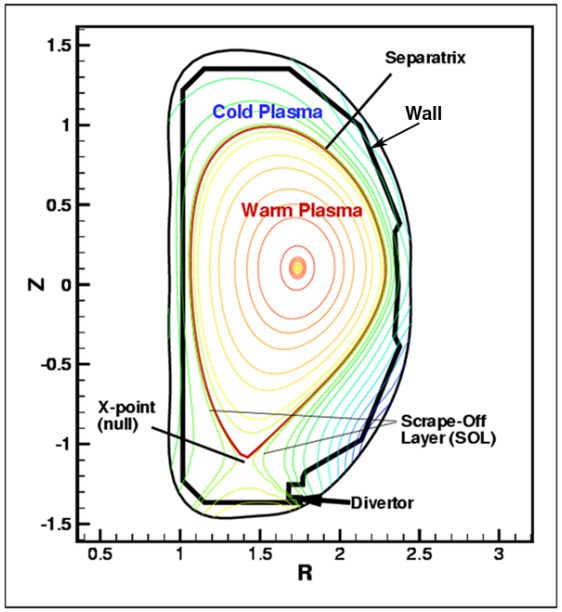


FACETS: Framework Application for Core-Edge Transport Simulations

- https://facets.txcorp.com/facets
- PI: John Cary, Tech-X Corporation

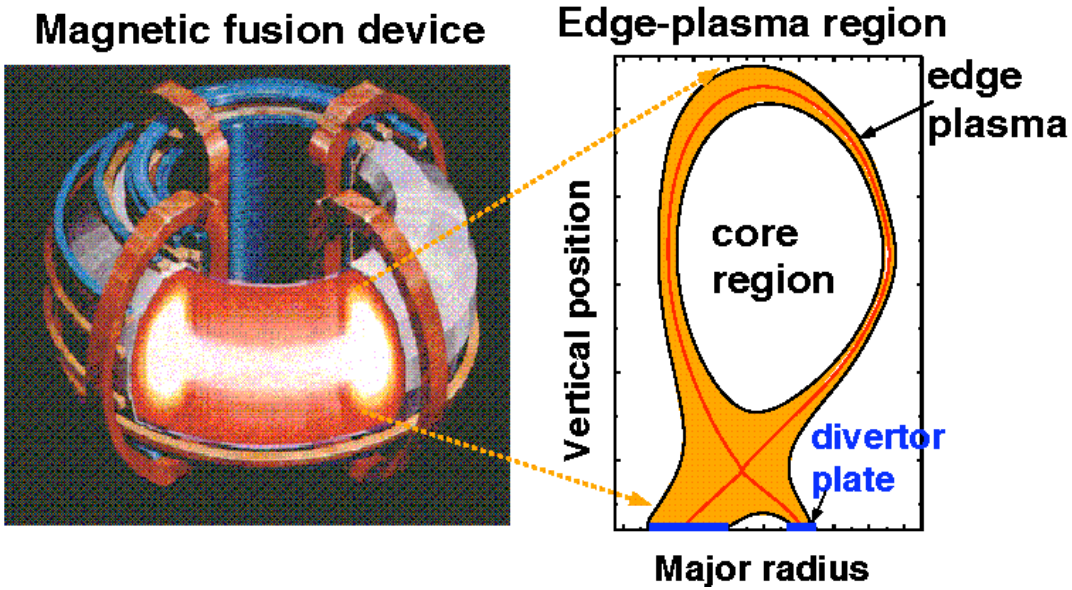
- Goal: Providing modeling of a fusion device from the core to the wall

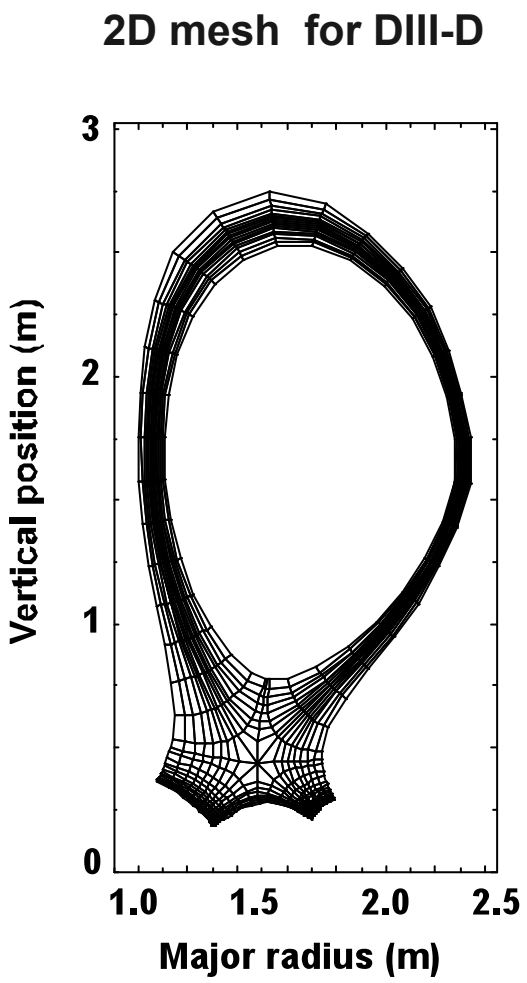
- TOPS Emphasis in FACETS
  - Incorporate TOPS expertise in scalable nonlinear algebraic solvers into the base physics codes that provide the foundation for the coupled models
  - Study mathematical challenges that arise in coupled core-edge and transport-turbulence systems



The edge-plasma region is a key component to include for integrated modeling of fusion devices

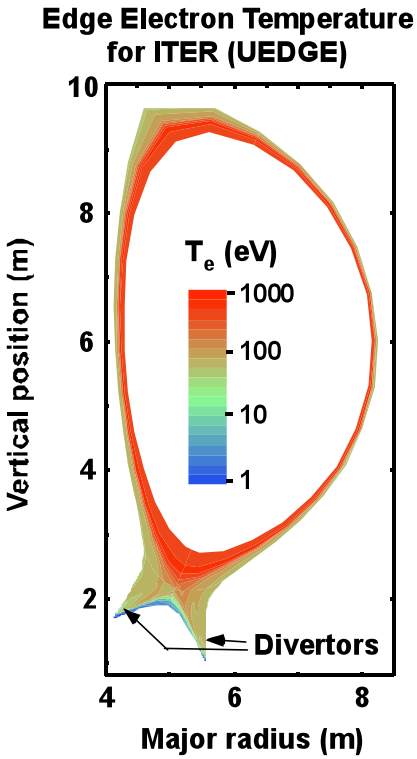
- Edge-pedestal temperature has large impact on fusion gain
- Plasma exhaust can damage walls
- Impurities from wall can dilute core fuel and radiate substantial energy





UEDGE is a 2D plasma/neutral transport code

- Features of UEDGE
  - **Physics:**
    - *Multispecies plasma; var. $n_{i,e}$, $u_{||i,e}$, $T_{i,e}$ for particle density, parallel momentum, and energy balances*
    - *Reaction-diffusion-convection type eqstions*
    - *Reduced Navier-Stokes or Monte Carlo for wall-recycled/sputtered neutrals*
    - *Multi-step ionization and recombination*
  - **Numerics:**
    - *Finite-volume discretization*
    - *Preconditioned Newton-Krylov implicit solver*
    - *Non-orthogonal mesh for fitting divertor*
    - *Steady-state or time dependent*
    - *Parallel version*
    - *PYTHON or BASIS scripting control*



References:

• T. D. Rognlien and M. E. Rensink, Edge-Plasma Models and Characteristics for Magnetic Fusion Energy Devices, *Fusion Engineering and Design,* 60: 497-514, 2002.

• T. D. Rognlien, D. D. Ryutov, N. Mattor, and G. D. Porter, Two-Dimensional Electric Fields and Drifts Near the Magnetic Separatrix in Divertor Tokamaks, *Physics of Plasmas*, 6 (5): 1851-1857, 1999.

• T. D. Rognlien, X. Q. Xu, and A. C. Hindmarsh, Application of Parallel Implicit Methods to Edge-Plasma Numerical Simulations, *Journal of Computational Physics*, 175: 249-268, 2002.

Outline

- Overview of PETSc
  - Linear solver interface: KSP
  - Nonlinear solver interface: SNES
  - Profiling and debugging
- Ongoing research and developments

The PETSc Programming Model

- Distributed memory, “shared-nothing”
  - *Requires only a standard compiler*
  - *Access to data on remote machines through MPI*
- Hide within objects the details of the communication
- User orchestrates communication at a higher abstract level than direct MPI calls

Getting Started

```
PetscInitialize();
ObjCreate(MPI_comm,&obj);
ObjSetType(obj, );
ObjSetFromOptions(obj, );

ObjSolve(obj, );
ObjGetxxx(obj, );

ObjDestroy(obj);
PetscFinalize()
```

PETSc Numerical Components

Nonlinear Solvers (SNES)		
Newton-based Methods		Other
Line Search	Trust Region	

Time Steppers (TS)			
Euler	Backward Euler	Pseudo Time Stepping	Other

Krylov Subspace Methods (KSP)							
GMRES	CG	CGS	Bi-CG-STAB	TFQMR	Richardson	Chebychev	Other

Preconditioners (PC)						
Additive Schwartz	Block Jacobi	Jacobi	ILU	ICC	LU (Sequential only)	Others

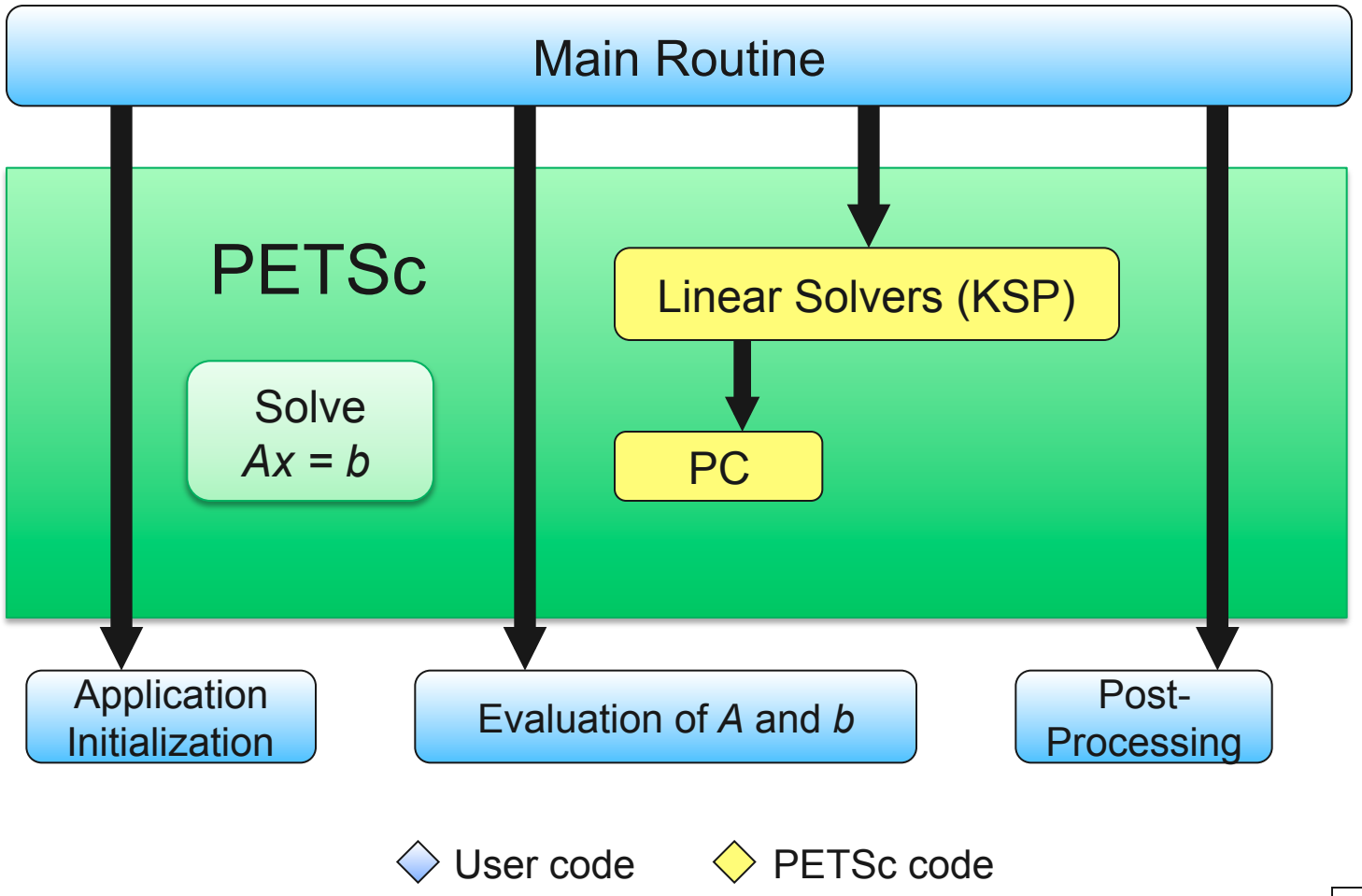
Matrices (Mat)					
Compressed Sparse Row (AIJ)	Blocked Compressed Sparse Row (BAIJ)	Block Diagonal (BDIAG)	Dense	Matrix-free	Other

Distributed Arrays(DA)

Index Sets (IS)			
Indices	Block Indices	Stride	Other

Vectors (Vec)

Linear Solver Interface: KSP



beginner

solvers: linear

Setting Solver Options at Runtime

- -ksp_type [cg,gmres,bcgs,tfqmr,…]
- -pc_type [lu,ilu,jacobi,sor,asm,…]

1

- -ksp_max_it <max_iters>
- -ksp_gmres_restart <restart>
- -pc_asm_overlap <overlap>
- -pc_asm_type [basic,restrict,interpolate,none]
- etc ...

2

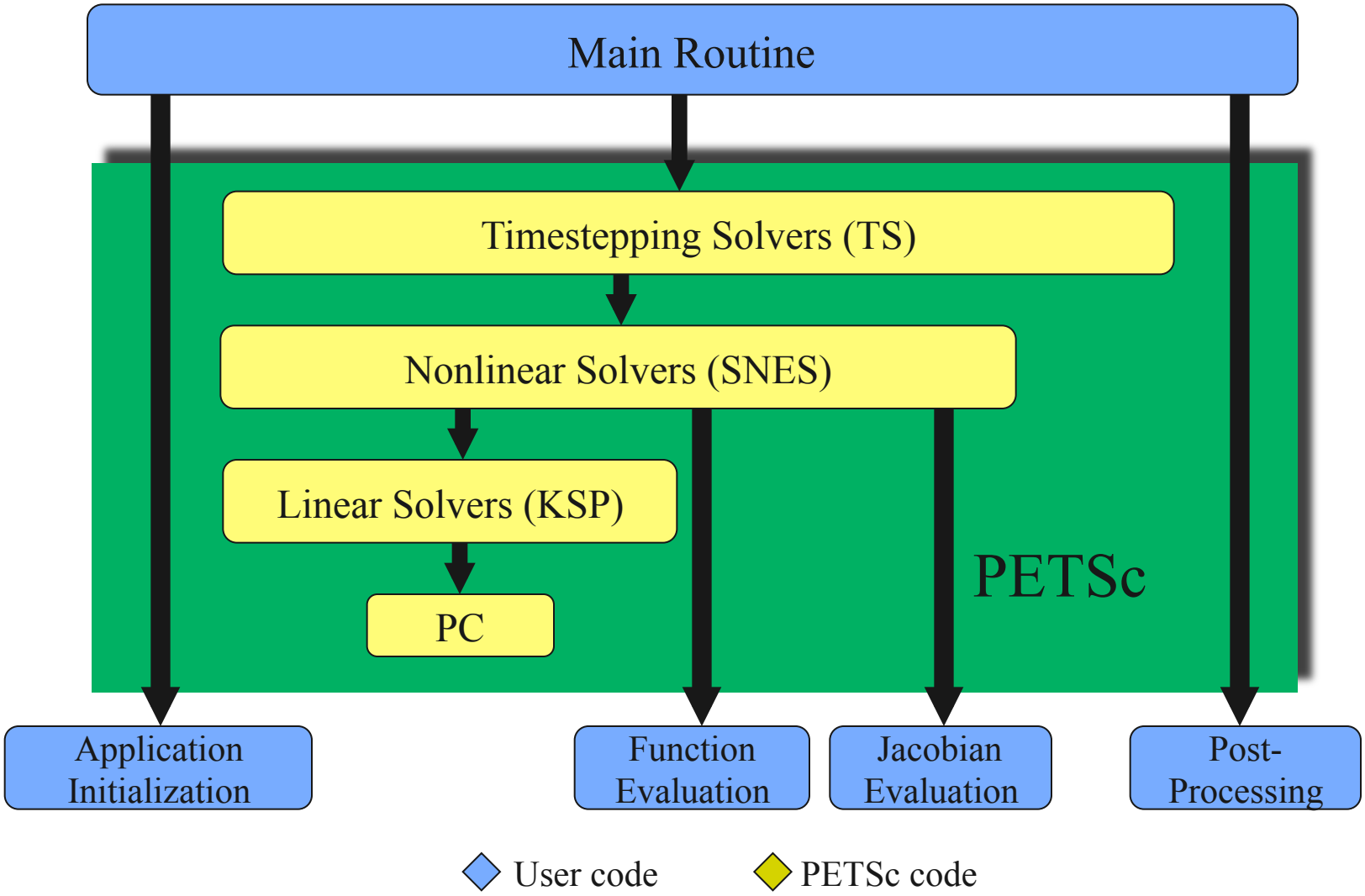
1 beginner | 2 intermediate

solvers: linear

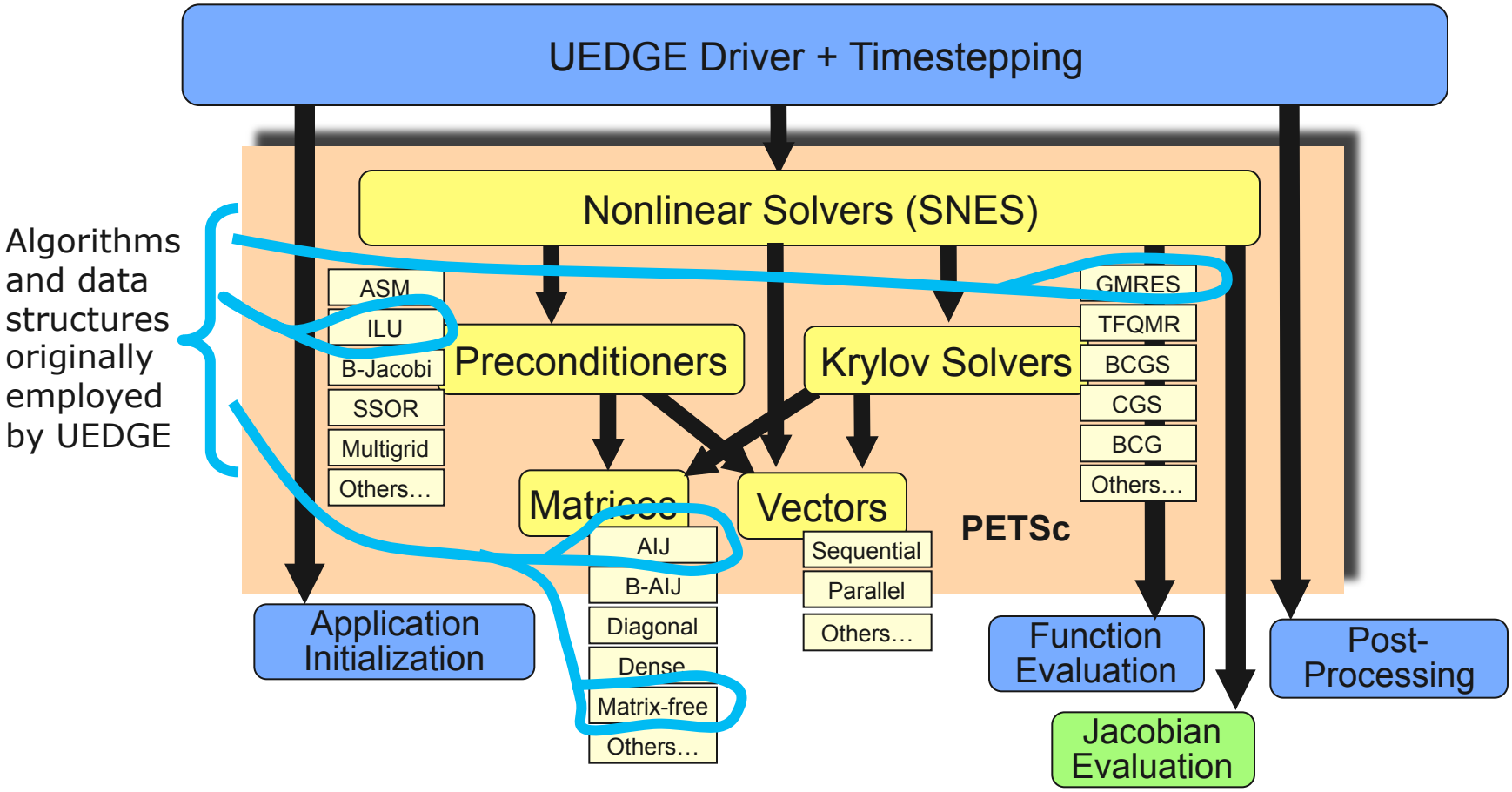
Recursion: Specifying Solvers for Schwarz Preconditioner Blocks

- Specify KSP solvers and options with "-sub" prefix, e.g.,
  - Full or incomplete factorization
    - *-sub_pc_type lu*
    - *-sub_pc_type ilu -sub_pc_ilu_levels <levels>*
  - Can also use inner Krylov iterations, e.g.,
    - *-sub_ksp_type gmres -sub_ksp_rtol <rtol>*
    - *-sub_ksp_max_it <maxit>*

Flow of Control for PDE Solution



Example (UEDGE): Solve F(u) = 0



Nonlinear Solver Interface: SNES

Goal: For problems arising from PDEs, support the general solution of $F(u) = 0$

User provides:

- Code to evaluate $F(u)$
- Code to evaluate Jacobian of $F(u)$ (optional)
  - *or use sparse finite difference approximation*
  - *or use automatic differentiation*
    - AD support via collaboration with P. Hovland and B. Norris
    - Coming in next PETSc release via automated interface to ADIFOR and ADIC (see http://www.mcs.anl.gov/autodiff)

SNES: Review of Basic Usage

SNESCreate( )	- Create SNES context
SNESSetFunction( )	- Set function eval. routine
SNESSetJacobian( )	- Set Jacobian eval. routine
SNESSetFromOptions( )	- Set runtime solver options for [SNES,SLES, KSP,PC]
SNESSolve( )	- Run nonlinear solver
SNESView( )	- View solver options actually used at runtime (alternative: -snes_view)
SNESDestroy( )	- Destroy solver

solvers: nonlinear

Uniform access to all linear and nonlinear solvers

- -ksp_type [cg,gmres,bcgs,tfqmr,…]
- -pc_type [lu,ilu,jacobi,sor,asm,…]
- -snes_type [ls,…]

- -snes_line_search <line search method>
- -sles_ls <parameters>
- -snes_convergence <tolerance>
- etc...

solvers: nonlinear

PETSc Programming Aids

- Correctness Debugging
  - Automatic generation of tracebacks
  - Detecting memory corruption and leaks
  - Optional user-defined error handlers
- Performance Profiling
  - Integrated profiling using -log_summary
  - Profiling by stages of an application
  - User-defined events

Ongoing Research and Developments

- Framework for unstructured meshes and functions defined over them
- Framework for multi-model algebraic system
- Bypassing the sparse matrix memory bandwidth bottleneck
  - Large number of processors (nproc =1k, 10k,…)
  - Peta-scale performance
- Parallel Fast Poisson Solver
- More TS methods
- …

Framework for Meshes and Functions Defined over Them

- The PETSc DA class is a topology and discretization interface.
  - Structured grid interface
    - *Fixed simple topology*
  - Supports stencils, communication, reordering
    - *Limited idea of operators*

- The PETSc Mesh class is a topology interface
  - Unstructured grid interface
    - *Arbitrary topology and element shape*
  - Supports partitioning, distribution, and global orders

- The PETSc DM class is a hierarchy interface.
  - Supports multigrid
    - *DMMG combines it with the MG preconditioner*
  - Abstracts the logic of multilevel methods

- The PETSc Section class is a function interface
  - Functions over unstructured grids
    - *Arbitrary layout of degrees of freedom*
  - Supports distribution and assembly

Parallel Data Layout and Ghost Values: Usage Concepts

Managing field data layout and required ghost values is the key to high performance of most PDE-based parallel programs.

Mesh Types

- Structured
  - DA objects
- Unstructured
  - VecScatter objects

Usage Concepts

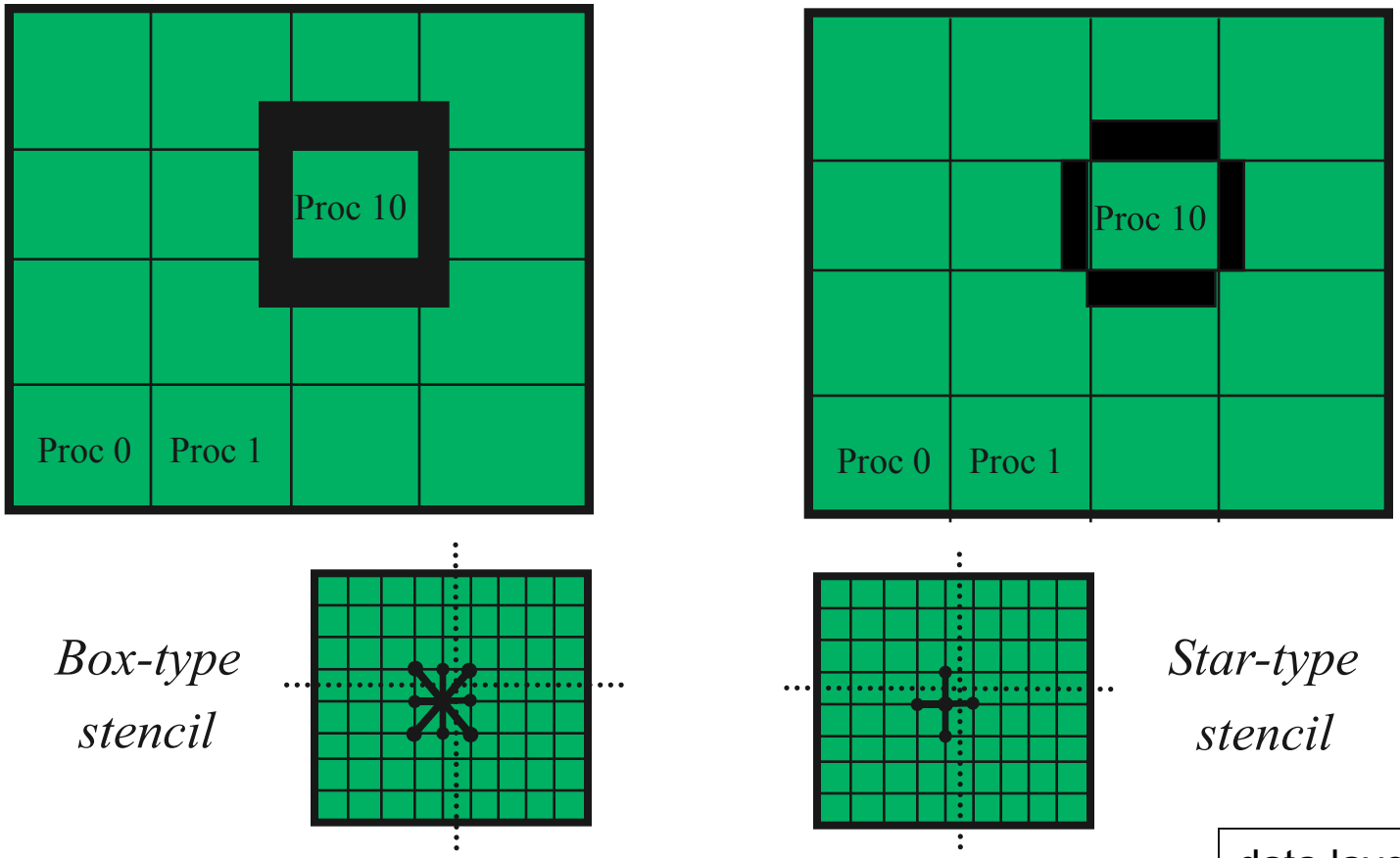
- Geometric data
- Data structure creation
- Ghost point updates
- Local numerical computation

important concepts

data layout

Distributed Arrays

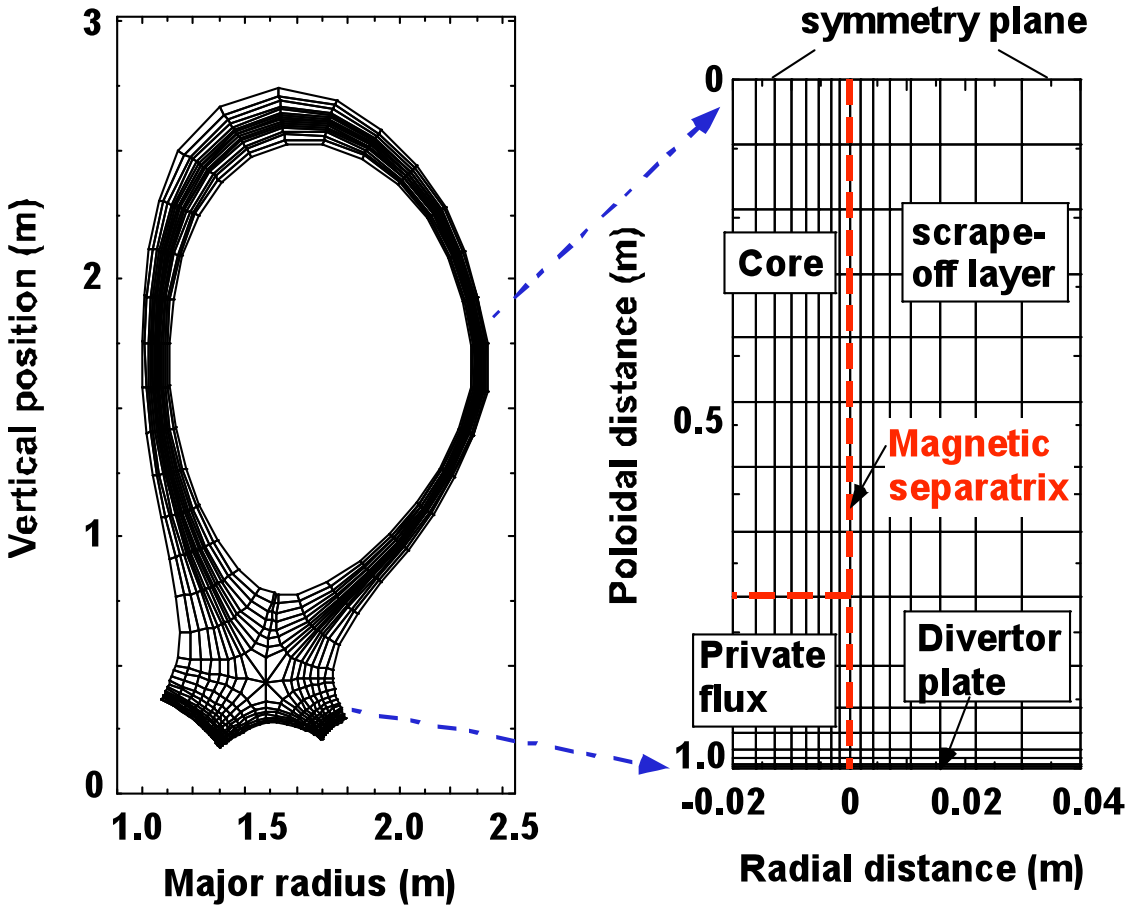
Data layout and ghost values



data layout:
distributed arrays

Full toroidal geometry is typically used, but initial parallel UEDGE tests with PETSc in equivalent slab

- Outer midplane/ divertor regions are mapped to an equivalent slab
- Same features such as closed and open B-field lines, private flux region, and divertor recycling are retained



Creating a DA

DACreate2d(comm, wrap, type, M, N, m, n, dof, s, lm[], ln[], *da)

wrap: Specifies periodicity

DA_NONPERIODIC, DA_XPERIODIC, DA_YPERIODIC, …

type: Specifies stencil

DA_STENCIL_BOX, DA_STENCIL_STAR

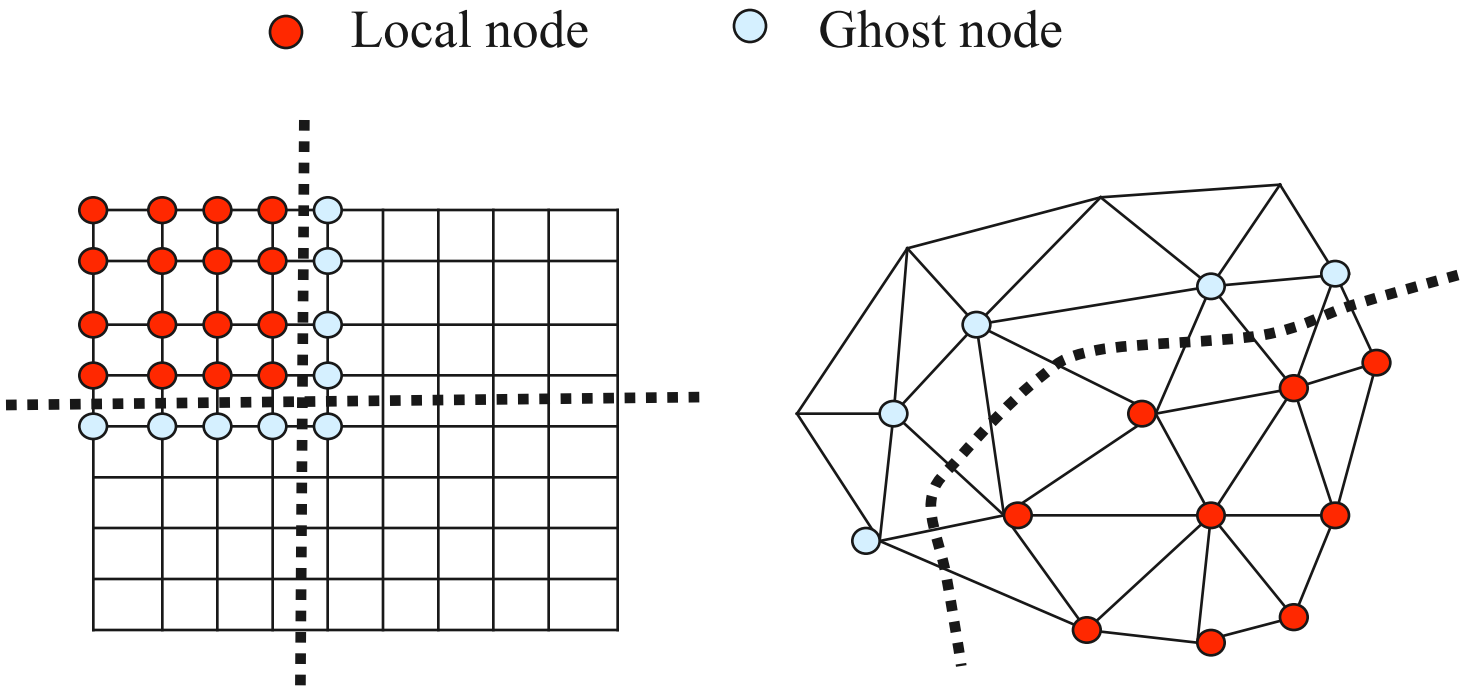
M/N: Number of grid points in x/y-direction

m/n: Number of processes in x/y-direction

s: The stencil width

lm/ln: Alternative array of local sizes

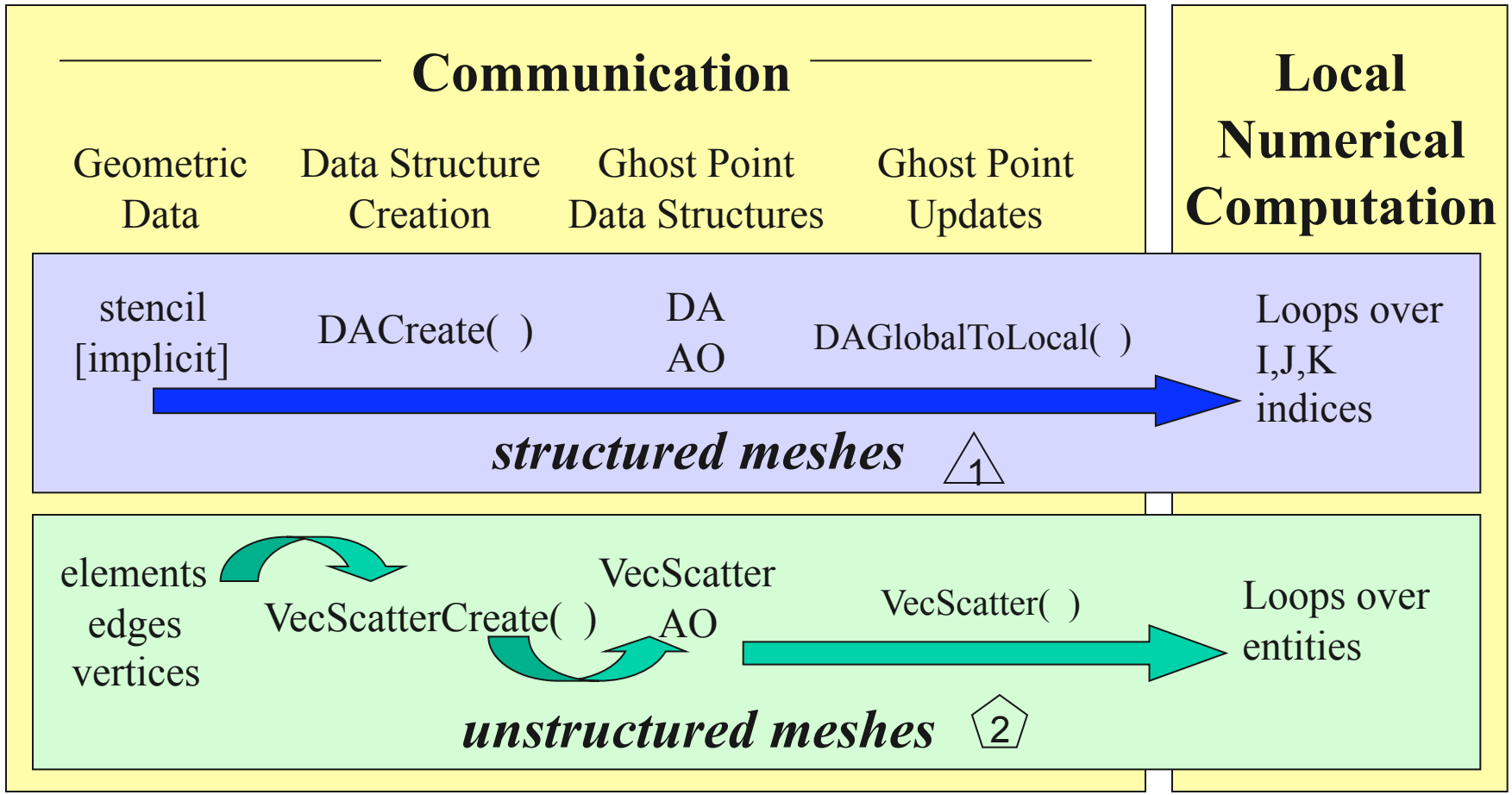
Ghost Values



To evaluate a local function $f(x)$, each process requires

- its local portion of the vector x
- its **ghost values** – bordering portions of x owned by neighboring processes.

Communication and Physical Discretization



A DA is more than a Mesh

A DA contains

topology, geometry, and an implicit Q1 discretization

It is used as a template to create

- Vectors (functions)
- Matrices (linear operator)

Creating the Mesh

- Generic object
  - MeshCreate()
  - MeshSetMesh()
- File input
  - MeshCreatePCICE()
  - MeshCreatePyLith()
- Generation
  - MeshGenerate()
  - MeshRefine()
  - ALE: :MeshBuilder::createSquareBoundary
- Representation
  - ALE::SieveBuilder::buildTopology()
  - ALE::SieveBuilder::buildCoordinates()
- Partitioning and distribution
  - MeshDistribute()
  - MeshDistributeByFace()

Parallel Sieves

- Sieves use names, not numberings
  - Numberings can be constructed on demand
- Overlaps relate names on different processes
  - An overlap can be encoded by a Sieve
- Distribution of a Section pushes forward along the Overlap
  - Sieves are distributed as “cone” sections

Sections associate data to submeshes

- Name comes from section of a fiber bundle
  - Generalizes linear algebra paradigm
- Define restrict(), update()
- Define complete()
- Assembly routines take a Sieve and several Sections
  - This is called a Bundle

Section Types

Section can contain arbitrary values

- C++ interface is templated over value type
- C interface has two value types
  - SectionReal
  - SectionInt

Section can have arbitrary layout

- C++ interface can place unknowns on any Mesh entity (Sieve point)
  - Mesh::setupField() parametrized by Discretization and BoundaryCondition
- C interface has default layouts
  - MeshGetVertexSectionReal()
  - MeshGetCellSectionReal()

Section Assembly

First we do local operations:

- Loop over cells
- Compute cell geometry
- Integrate each basis function to produce an element vector
- Call SectionUpdateAdd()

Then we do global operations:

- SectionComplete() exchanges data across overlap
  - *C just adds nonlocal values (C++ is flexible)*
- C++ also allows completion over arbitrary overlap

Framework for Multi-model Algebraic System

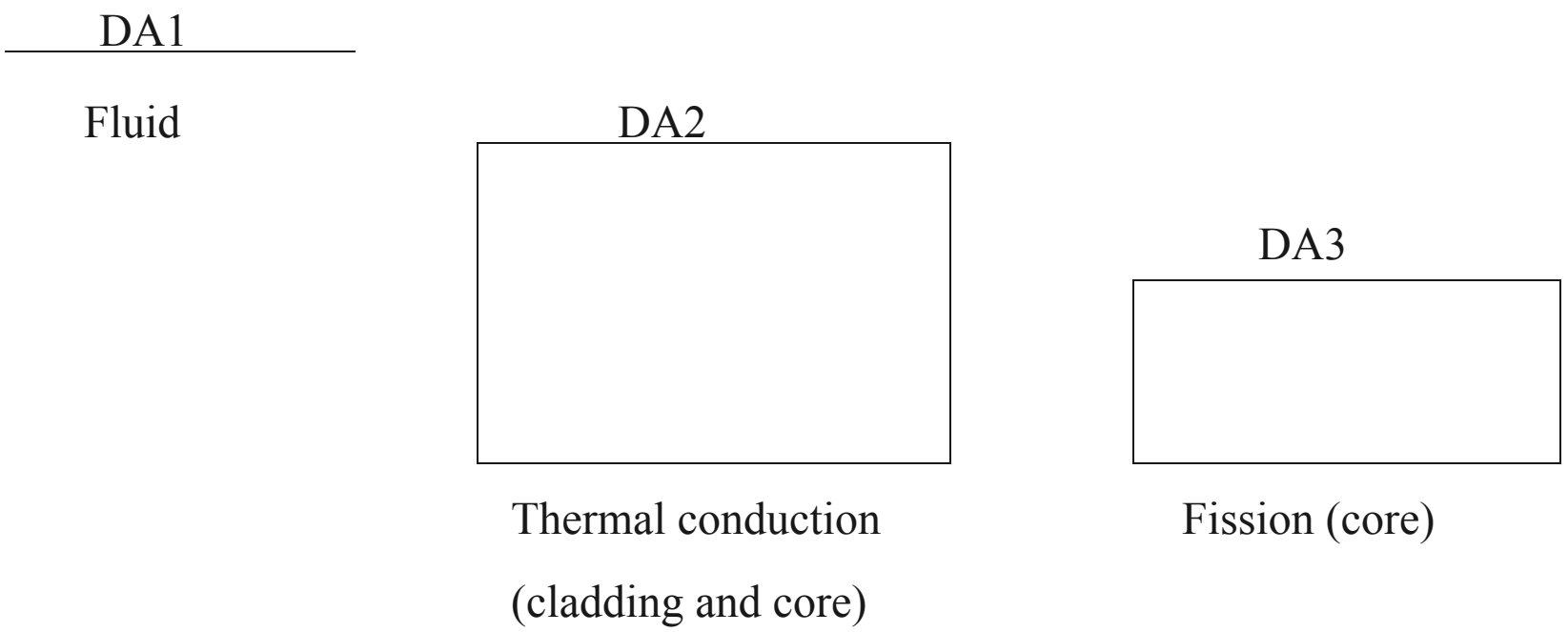
~petsc/src/snes/examples/tutorials/ex31.c, ex32.c

http://www-unix.mcs.anl.gov/petsc/petsc-as/snapshots/petsc-dev/tutorials/multiphysics/tutorial.html

Framework for Multi-model Algebraic System
~petsc/src/snes/examples/tutorials/ex31.c

A model "multi-physics" solver based on the Vincent Mousseau's reactor core pilot code:

There are three grids



```
/* Create the DMComposite object to manage the three grids/physics. */
DMCompositeCreate(app.comm,&app.pack);
DACreate1d(app.comm,DA_XPERIODIC,app.nxv,6,3,0,&da1);
DMCompositeAddDA(app.pack,da1);
DACreate2d(app.comm,DA_YPERIODIC,DA_STENCIL_STAR,…,&da2);
DMCompositeAddDA(app.pack,da2);
DACreate2d(app.comm,DA_XYPERIODIC,DA_STENCIL_STAR,…,&da3);
DMCompositeAddDA(app.pack,da3);

/* Create the solver object and attach the grid/physics info */
DMMGCreate(app.comm,1,0,&dmmg);
DMMGSetDM(dmmg,(DM)app.pack);
DMMGSetSNES(dmmg,FormFunction,0);

/* Solve the nonlinear system */
DMMGSolve(dmmg);

/* Free work space */
DMCompositeDestroy(app.pack);
DMMGDestroy(dmmg);
```

```
/* Unwraps the input vector and passes its local ghosted pieces into the user
      function */
FormFunction(SNES snes,Vec X,Vec F,void *ctx)
…
DMCompositeGetEntries(dm,&da1,&da2,&da3);
DAGetLocalInfo(da1,&info1);

/* Get local vectors to hold ghosted parts of X;
   then fill in the ghosted vectors from the unghosted global vector X */
DMCompositeGetLocalVectors(dm,&X1,&X2,&X3);
DMCompositeScatter(dm,X,X1,X2,X3);

/* Access subvectors in F - not ghosted and directly access the memory
      locations in F */
DMCompositeGetAccess(dm,F,&F1,&F2,&F3);

/* Evaluate local user provided function */
FormFunctionLocalFluid(&info1,x1,f1);
FormFunctionLocalThermal(&info2,x2,f2);
FormFunctionLocalFuel(&info3,x3,f3);
```

Bypassing the Sparse Matrix Memory Bandwidth Bottleneck

- Newton-multigrid provides
  - good nonlinear solver
  - easy utilization of software libraries
  - low computational efficiency
- Multigrid-Newton provides
  - good nonlinear solver
  - lower memory usage
  - potential for high computational efficiency
  - requires “code generation/in-lining”

- Parallel Fast Poisson Solver
- More TS methods
- …

How will we solve numerical applications in 20 years?

- Not with the algorithms we use today?
- Not with the software (development) we use today?

How Can We Help?

- Provide documentation:
  - http://www.mcs.anl.gov/petsc
- Quickly answer questions
- Help install
- Guide large scale flexible code development
- Answer email at petsc-maint@mcs.anl.gov