Frameworks for Modeling and Inversion

William W. Symes

The Rice Inversion Project

Department of Computational and Applied Mathematics
Rice University, Houston, TX

symes@caam.rice.edu

Project Goal:

Aid rapid prototyping of new wave modeling, inversion apps – wave physics, modeling methods, optimization algorithms, hardware & software environments –

without starting from scratch every time

Find the right abstractions and data structures, create a proof-of-concept open source implementation

Components

- Modeling – IWAVE
- Optimization – RVL
- Inversion – IWAVE++

Framework for Wave Modeling [IWAVE]

Why a framework?

- FD, FE apps share many common tasks:
  - Grid allocation
  - Data exchange patterns (domain decomposition) – depend on scheme
  - i/o w. common file structures (SEGY/SU, RSF,…)
- Many of these reusable across many apps, given interfaces and task def'ns
- Unstructured-mesh FEM frameworks (mostly CFD-oriented): PETSc, DUNE, deal.II, FEniCS, Trilinos,…
- Regular grid FD/FE TD: restricted domain - additional opportunities for re-use, efficient implementation

Basic Data Structures for FDTD

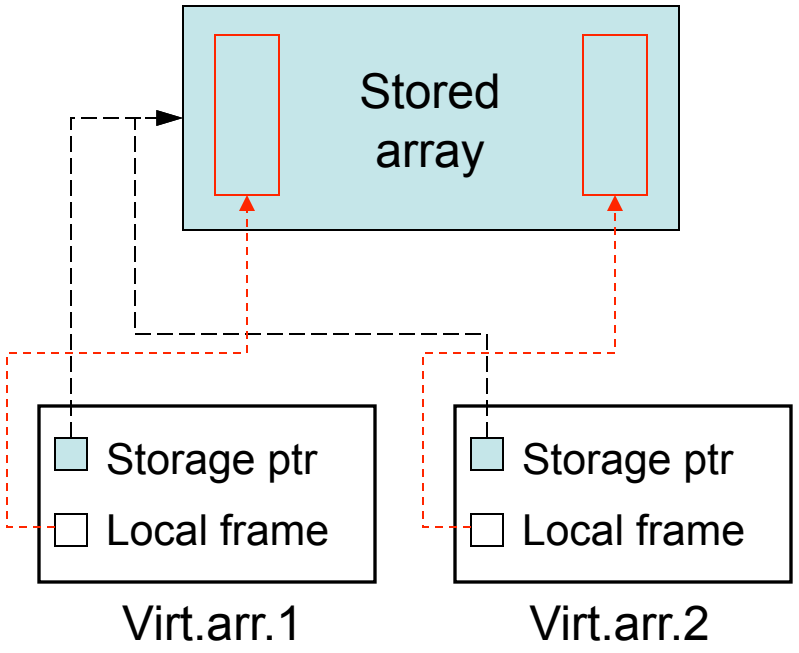
Regular grid methods: Arrays = fcns on rectangular subsets of infinite lattice, virtual sub-arrays

• Every virtual sub-array carries reference to parent allocated array
• Arrays located relative to common lattice – can compute overlaps, data exchanges,…

State of system = union of static, dynamic arrays, with functions: constructors, data exchange, time updates

Source, receiver data: arbitrary locations, position relative to reference lattice, sampling & i/o

[IST, TRIP 2008]



Methods:

- Create/resize subarrays
- Output
- Etc.

Our Implementation: IWAVE

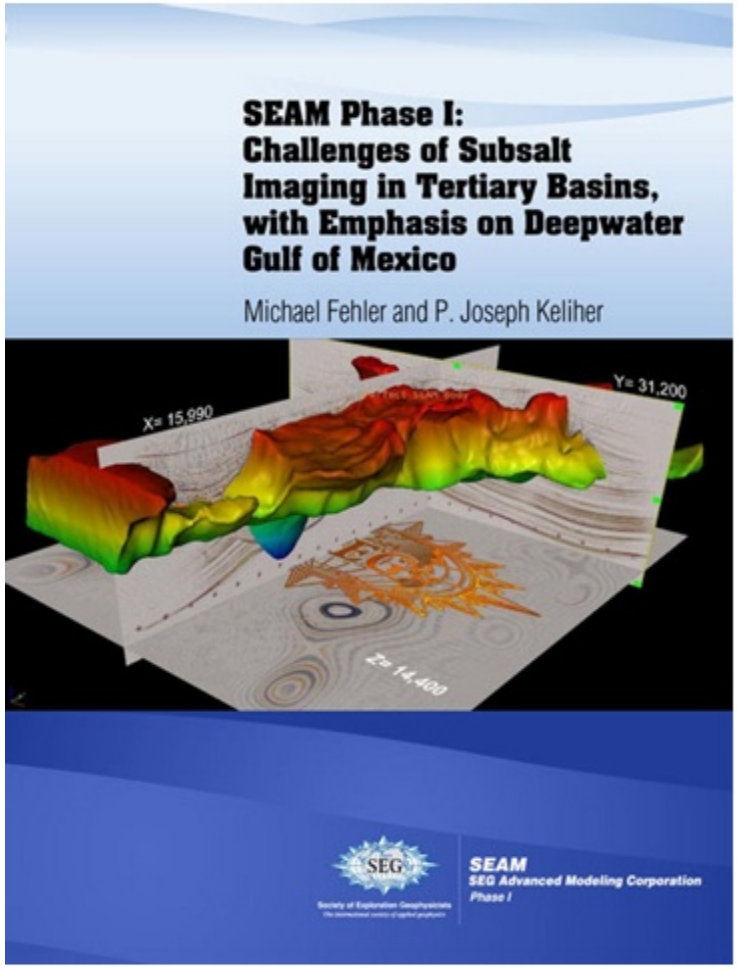
- ISO C99
- “Object oriented C”: built around small set of C structs containing data and functions operating on them
- Core modules: services – memory, comm, i/o, job control
- State repn = `RDOM` = array of arrays
- State type = `IMODEL` – struct with `RDOM` and many virtual sub-RDOMS, functions eg.

```
tsf(RDOM * p, int * iv, void * pars)
```

- Application modules (“apps”) – choices of physics, scheme
- Parallelism via domain decomposition, MPI.
- Reads, writes data in standard exchange formats: initially SEGY/SU, RSF,…
- Open source, X11 license

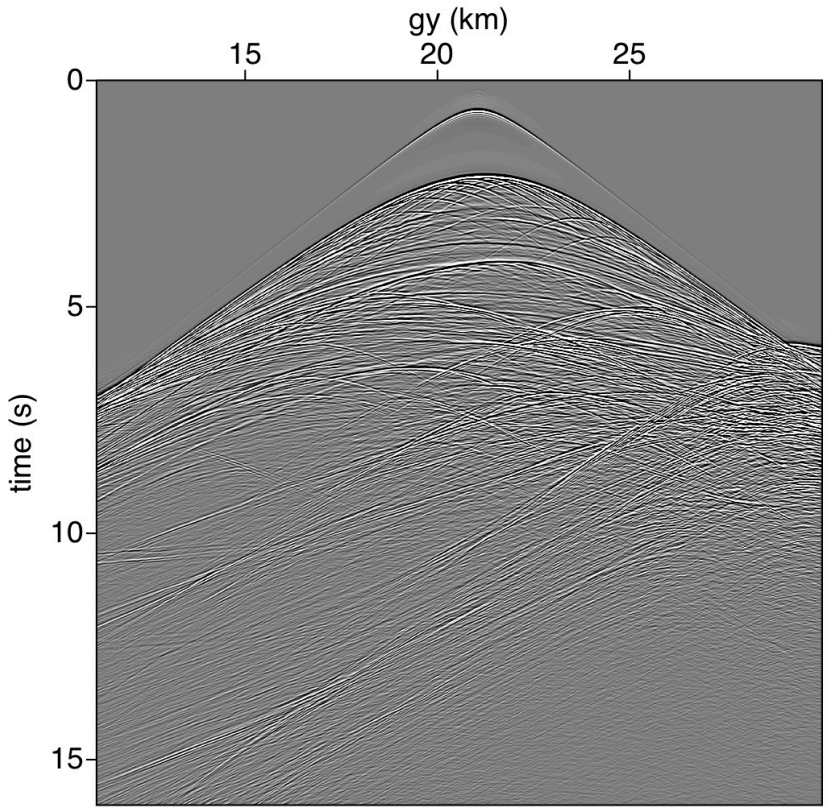
IWAVE & SEAM Phase I

- Public domain QC code – high accuracy FDTD, ABCs, SEAM-sized data, scale to 1000's of cores
- Couldn't find one, so we built it
- For the details: new SEG e-book by Fehler & Keliher - many insights into project management, QC – role of IWAVE



Visual Comparison: Shot 20433, E-W line at N 10.585 km

Tierra



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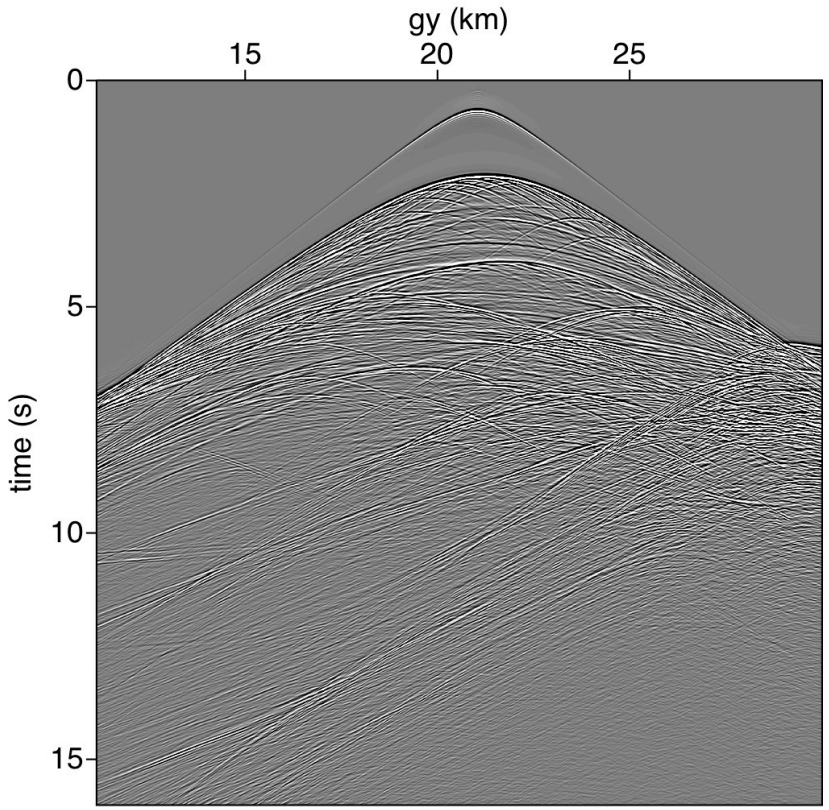
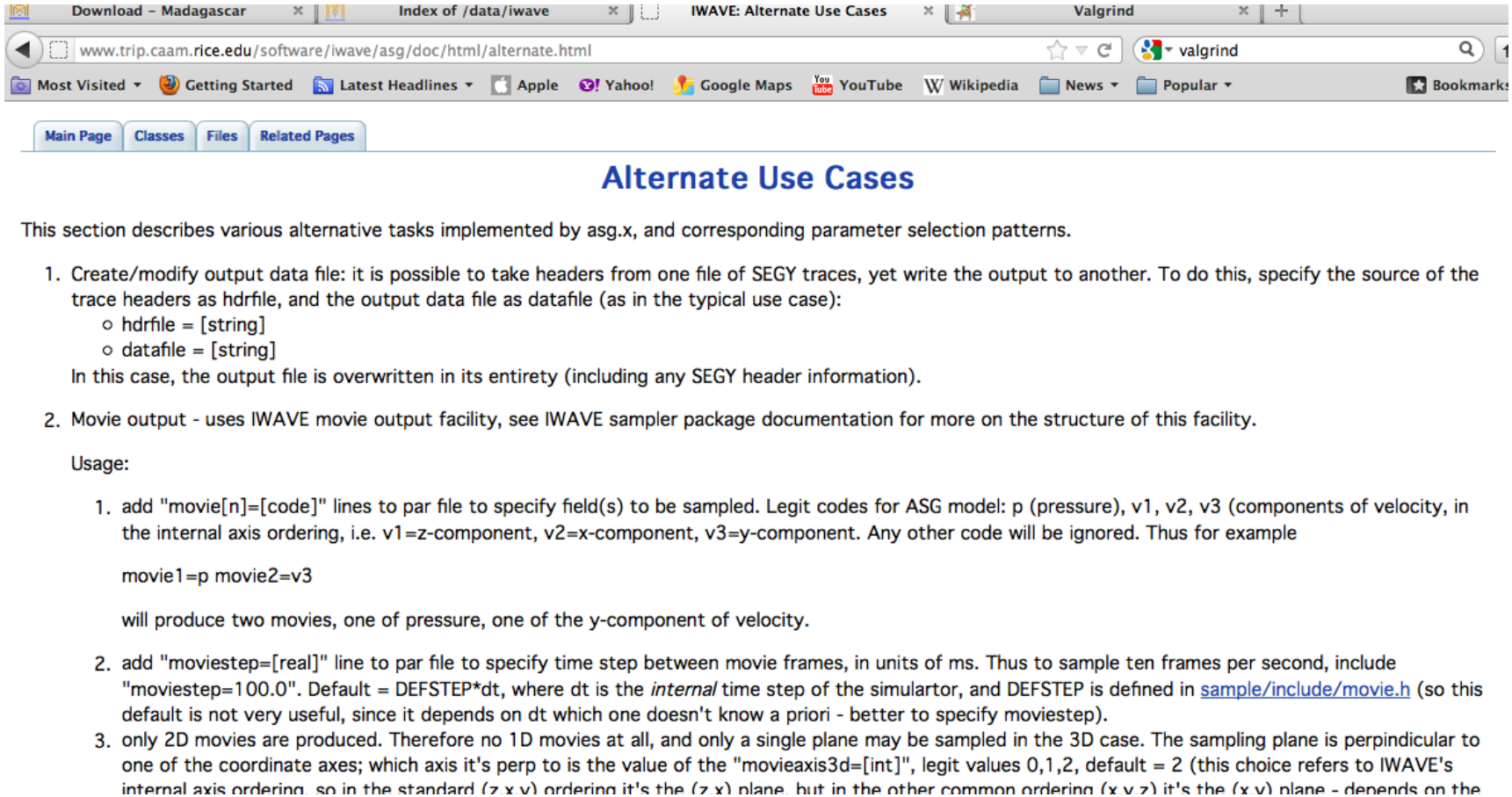
IWAVE



IWAVE Documentation



Abstract Optimization and Linear Algebra [Rice Vector Library]

Types for Abstract Optimization

Essential step: define types for high level abstractions – Space, Vector, (linear or nonlinear) Operator, Functional

Evaluation objects – organize the value of function & derivatives at a point, enforce coherency

With these, can express coordinate free algorithms of linear algebra and optimization – Krylov (CG etc.), Lanczos, Landweber, quasi-Newton,…

Our Implementation: the Rice Vector Library ("RVL")

C++ classes expressing calculus in Hilbert Space

Design Paper: Padula, Scott & S, ACM TOMS 2009

Standard interfaces to concrete data types – in-core, out-of-core, distributed,… - and operations on them:

- `DataContainer` – data abstraction, forms Visitor pattern with
- `FunctionObject` – encapsulates all actions on data

Abstract Optimization with RVL

Typical use: RTM looks like

```
MyKindaDataSpace dsp(…);
MyKindaModelSpace msp(…);
Vector m(msp); Vector g(msp); Vector d(dsp);
…
MyKindaModelingOp op(….);
OperatorEvaluation opeval(op,m);
opeval.getDeriv().applyAdj(d,g);
```

"THE MATH IS THE API"

Abstract Optimization with RVL

Built on RVL:

Optimization Library `UMin`: LBFGS, trust region G-N-K, CG, Arnoldi…

Abstract time-stepping library `TSOpt`, including universal implementation of optimal checkpointing (Griewank 92)

Plans: additional algorithms (L1, TV, TR-SQP, …)

Inversion
[RVL + IWAVE = IWAVE++]

Requirements for inversion implementations

- modeling:
  - forward modeling
  - linearized (“Born”) modeling
  - adjoint (transposed) linearized modeling
- optimization algorithm, implementation
- interface between modeling and optimization

Natural type mismatch between modeling & optimization – concrete (grids, traces) vs. abstract (vectors, operators)

Internal state of simulator need not be a Vector object – only input and output types

Our Solution: IWAVE++

Middleware layer – C++ classes encapsulating

- input & output types for IWAVE as RVL vector classes
- out-of-core design
- Born & adjoint extensions of IWAVE function interfaces, eg.

```
tsfa(RDOM * p, RDOM * r, int iv, void * pars)
```

- delegates time loop control, checkpointing to TSOpt

Defines abstract RVL Operator class combining fwd, lin, and adj modeling

[WWS, Enriquez & Sun, Geophys. Prosp. 11]

Our Implementation: IWAVE++

Simple expl – adjoint (“dot product”) test

```
IWaveOp<(list of policy types)> op(dom, rng, pars, stream,
minit);
Vector<float> m(op.getDomain());
… (initialize m)…
OperatorEvaluation<float> opeval(op,m);
AdjointTest(opeval.getDeriv(), rnd, stream);
```

Output, Marmousi 4m grid, 960 cores, 4x1 dom decomp:

adjoint relation holds:|<Ax,y>-<x,A'y>|/|Ax||y| = 4.91893895e-12
< 100*macheps = 1.19209290e-05
<Ax,y> = -1.63633438e+05
<x,A'y> = -1.63633469e+05
|Ax||y| = 6.35299635e+09

Releases and Availability

Releases, plans

- IWAVE:
  - initial release at SEG 09
  - initial through current (1.5) at TRIP web site www.trip.caam.rice.edu
  - beginning with next release (2.0, 12 Q3) at SourceForge svn rsf.svn.sourceforge.net/svnroot/rsf/trunk
  - download and install either
    - stand-alone, or
    - integrated with Madagascar
- RVL:
  - initial release 11 Q3
  - r1.2 coming 12 Q3
- IWAVE++:
  - beta
  - Initial release planned for early 13

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- IWAVE team – Igor Terentyev, Tanya Vdovina, Xin Wang
- RVL team – Mark Gockenbach, Shannon Scott, Tony Padula, Hala Dajani
- IWAVE++ team - Dong Sun, Marco Enriquez
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www.trip.caam.rice.edu/software