Computational Economics: Practical Tools and Techniques
Scientific computing (cont.)

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Key points (review)

- Types of computing: commercial software development vs. scientific research
- From real analysis to numerical methods and computing
- Computer architecture: from naive serial code to vectorization and parallelization
- Low-level tools and techniques: programming languages, math libraries, interactive agile prototyping, high performance computing
- High-level tools and techniques: non-linear and linear optimizers, using domain knowledge for efficient computing
- Parallel programming concepts
- Massively parallel processors $\Rightarrow$ simpler numerical algorithms: larger block-independent data frames with optimal function calls
- All modern CPUs are in a sense massively parallel processors!
- Hybrid computing: single-core HPC, multi-core and cluster computing, many core CPU-GPU and Intel MIC computing

Mapping research ideas to computer architecture

going back and forth between your model and computing implementation

- start mapping your model to computing architecture from the ground up
- single-core $\rightarrow$ representative optimizing agent with complex dynamics
- multi-core $\rightarrow$ heterogeneous independent agents processing different shocks under common information set
- fusion systems (clusters with Intel Phi co-processor, CPU-GPU) $\rightarrow$ hierarchical, multiscale models, micro founded macro models

Math libraries: from real analysis to computing

Implementation matters!

- Intel MKL: industry-standard, can be fine-tuned to use OpenMP, MPI efficiently
- OpenBLAS - multi-threaded high performance implementation for multi-core CPUs
- MacOS X: Accelerate framework
- MATLAB with Intel MKL $\Rightarrow$ 5-6 times faster than open source Fortran/BLAS
- The GNU Scientific Library (GSL) - a C replacement for numerical procedures written in Fortran (Netlib), NO high performance BLAS
- EIGEN templates and Armadillo C++ linear algebra library, the syntax (API) deliberately similar to MATLAB
- R computations with Intel MKL and automatic offloading to Intel Xeon Phi for big data

Scientific computing and business software development

- version control (subversion, git), unit tests, use cases
- modularity, reusability
- need to budget time and resources to comply with the best practices from business software development!
- what went wrong with C++
    - Arrays are not a core part of the language
    - Pointers are everywhere with random holes in memory lanes!
    - Some important features of Fortran-90 only 20 years later added as C/C++ extension in Intel Cilk Plus
- Java: dynamically allocated or resizable arrays $\Rightarrow$ very slow
- CS favorite objects (lists, maps, trees) and concepts (metaprogramming) are huge performance hogs
- Recursions and lambda-calculus $\Rightarrow$ hard to parallelize
- NumPy, MATLAB, FORTRAN - a view over the memory, strided memory model, fast performance lane, no slowing down due to OO design and random pointers

Non-linear Optimization with derivatives:

one solver does not fit all

- Gradients and Hessians are critical for Newton-based NL solvers
- Solution update method: Sequential Quadratic Programming (SQP), Interior-Point (IP)
- Global optimum: trust region, line search
- Penalty function, tolerance, feasibility
- SNOPT
  - line-search SQP; null-space CG option
  - l_1 exact penalty function
- IPOPT - open source in COIN-OR
  - line-search filter algorithm
- KNITRO
  - trust-region Newton, interior with CG option or direct
  - l_1 exact penalty function
  - Active Set - for medium size problems with good initial guess
- If your problem fails to be solved by IPOPT/SNOPT, it might be solved by KNITRO or vice versa

Optimization with weakened assumptions : abandoning convexity requirement!

domain knowledge $\Rightarrow$ efficient numerical algorithms

- MATLAB fminsearch

  Nelder-Mead Simplex (slow but reliable)

- Augmented Lagrangian methods (Arrow & Solow, 1958), method of multipliers (Hestens, Powell, 1969) $\Rightarrow$ Pattern Search

$$\underset{X}{\text{maximize}}\ f(X), s.t.\ h(X) = 0$$

  Lagrangian

$$\mathfrak{L}(X;\Lambda) = f(X) + \Lambda' h(X)$$

  Gradient process

$$\dot{X} = \mathfrak{L}_X(X;\Lambda); \dot{\Lambda} = \mathfrak{L}_\Lambda(X;\Lambda)$$

  Modified (augmented) Lagrangian (based on Lemma by Debreu, Econometrica (1952))

$$\mathfrak{L}(X;\Lambda|\theta) = f - \theta h' h + \Lambda' h;$$

  Gradient process

$$\dot{X} = f'_X - 2\theta h'_X h + h'_X \Lambda; \dot{\Lambda} = h$$

  or set $V = \Lambda + 2\theta\dot{\Lambda}$ then

$$\dot{X} = f'_X + h'_X V$$

  Λ represents current market price which rises or falls if excess demand is positive or negative.
  V a kind of expected price, based on extrapolation of current rates of change

- HOPSPACK (Hybrid Optimization Parallel Search PACKage)

  with asynchronous pattern search solver (supports MPI, OpenMP) over user-defined objective and nonlinear constraint functions (Fortran,C/C++, Perl, MATLAB, Python)

Numerical recipes and domain expertise:

textbook numerical recipes $\Rightarrow$ build up accurate domain guidance

"Redistribution and Social Insurance"
Mikhail Golosov, Maxim Troshkin, Aleh Tsyvinski, 2013.

- finite-horizon discrete-time dynamic programming problem with a three-dimensional continuous state space
- three-stage computational procedure
- shape-preserving least absolute deviation (LAD) value function iteration method with Chebyshev polynomials
- essential to have an efficient and robust optimization algorithm to solve mechanism design problems
- mechanism design problem is a bi-level maximization problem
- the outer-level maximization of the planner has to take into account the best response of the agents, which is the outcome of the inner-level maximization of each agent type with respect to the type reported
- implementation in AMPL/KNITRO
- interior-point optimization with CG iteration for inner-level, active-set with sequential linear quadratic programming iteration at outer level
- globalization strategy - explore multiple feasible starting points
- simple age-dependent linear taxes - welfare loss of 0.9% of consumption equivalent

"Insurance and Taxation over the Life Cycle"
Emmanuel Farhi and Ivan Werning, 2013. Review of Economic Studies, 80.

- It is surprising just how well this relatively simple policy performs. It delivers a welfare gain of 1.47% in lifetime consumption, compared to the 1.56% obtained by the second best. Remarkably, age-dependent linear taxes deliver 95% of the welfare gains of the second-best.
- our characterization of the second best, theoretical and numerical, provides not only useful insights, but can also deliver detailed and surprisingly accurate guidance for simpler tax systems

Non-convex problems: moral hazard and adverse selection

Su-Judd (2007), based on Alexander Karaivanov (2001): "Computing Moral Hazard Programs with Lotteries Using Matlab"

Part 1: Deterministic contract (non-linear program)

- Action-Output
  $\mathcal{A} \otimes \mathcal{Q} : \{a_1, ...a_{na}\} \otimes \{q_1, ...q_{nq}\}$
- Stochastic Production Function $p(q|a)$
- Compensation Schedule
  $\mathcal{C}(\mathcal{Q}) = \{c(q_1), ..., c(q_{nq})\}$
- Expected utility for the agents $\omega(c, a) = \sum_{q \in \mathcal{Q}} p(q|a)u(c(q), a)$

Deterministic contract (non-linear program)

Principal utility $\mathfrak{U}[q - c(a)]$, $q - c(a)$: net profit

$$\underset{(c,a)}{\text{maximize}} \sum_{q \in \mathcal{Q}} p(q|a)\mathfrak{U}[q - c(a)]$$
$$\text{s.t.}$$

Participation Constraints:

$$\omega(c, a) \geq \omega_0$$

Incentive Compatibility Constraints (ICC):

$$\omega(c, a) \geq \omega(c, \overline{a}),\ \forall \overline{a} \in \mathcal{A}$$

- Global optimum is not guaranteed
- Sensitive to starting conditions and choice of NL solver

Computing Moral Hazard Programs:

make the problem convex by using lotteries

Part 2: Prescott-Townsend Lotteries (linear program)

- Global optimum (conditional on the grid) is reliably achieved
$$\underset{\pi(q,c,a)}{\text{maximize}} \left[\sum_{\mathcal{Q},\mathcal{C},\mathcal{A}} \pi\left(q,c,a\right)\mathfrak{U}\left[q-c\right]\right]$$
- $\pi(q,c,a)$ is a probability distribution
- Participation Constraints:
$\sum_{\mathcal{Q},\mathcal{C},\mathcal{A}} \pi\left(q,c,a\right) u\left(c,a\right) \geq u_0$
- Mother Nature/Technology Constraints:
$\forall \left\{\overline{q},\overline{a}\right\} \in \mathcal{Q}\times\mathcal{A}$
$\sum_{\mathcal{C}} \pi(\overline{q},c,\overline{a}) = P\left(\overline{q}|\overline{a}\right)\sum_{\mathcal{Q},\mathcal{C}} \pi(q,c,\overline{a})$
- Incentive Compatibility Constraints (ICC) for action variables:
$\forall\ a,\hat{a} \in \mathcal{A}\times\mathcal{A}$
$\sum_{\mathcal{Q},\mathcal{C}} \pi\left(q,c,a\right) u(c,a) \geq \sum_{\mathcal{Q},\mathcal{C}} \pi\left(q,c,a\right) \frac{P(q,\hat{a})}{P(q,a)} u(c,\hat{a})$

Linear Programming: the choice of solver matters

- MATLAB linprog
- Open source: GLPK, lp_solve, CLP, SoPlex
- IBM CPLEX , XPRESS
- Gurobi: Interfaces to R, MATLAB, Python
- reliable information is hard to find, obsolescence is an issue
- need to be aware before you know you need it

	running time	instances solved	solved (%)
CBC	10.20	41	47.13
CPLEX	1.45	73	83.91
GLPK	22.11	3	3.45
GUROBI	1.00	77	88.51
LP_SOLVE	19.40	5	5.75
SCIP-C	3.76	63	72.41
SCIP-L	6.40	52	59.77
SCIP-S	5.33	57	65.52
XPRESS	1.29	74	85.06

SCIP-L (using CLP);SCIP-S (using SoPlex)

"Analysis of commercial and free and open source solvers for linear optimization problems", B. Meindl and M. Templ, 2012.

Hybrid approach to Moral Hazard and Adverse Selection Programs

Su-Judd (2007)

- Step 1: Solve LP in lotteries on coarse grids which guarantees solution that can serve as a good starting point - close to global optimum
- Step 2: Use this information to exclude bad (nonsensical) local traps from non-linear constrained optimization
- Step 3: (locally convergent only!) Combine with multi-start option in non-linear solver to converge quickly on (hopefully) true global optimum
- Step 4: (optional) Iterate
- Step 5: (optional) Do Structural Estimation in parallel

Parallel Programming:

same task done faster or more complex task done in feasible time

SAXPY, single-precision real Alpha X Plus Y (BLAS, level 1):

$$Y \leftarrow \alpha * X + Y$$

where X_i, Y_i, $i \in [1, n]$ - vectors

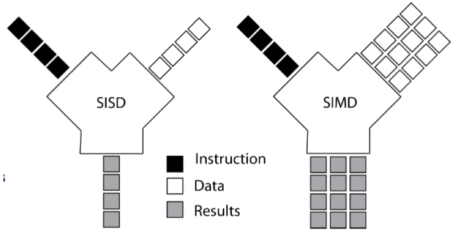
- Instruction (control) parallelism, strong scaling
  - Scalar uniprocessor - $2n$ steps
  - Two functional units (an adder and a multiplier) - $n + 1$ steps, speedup $\frac{2n}{n+1} \approx 2$
  - Amdahl's law:
    If s is a fraction of code that is executed serially then speedup from parallelizing $p = 1 - s$ fraction using N processors:

$$Speedup \leq \frac{1}{s + p/N}$$

- Data parallelism: two steps with n processors handling $\alpha * X$ and Y simultaneously, speedup is proportional to $N < n$
- Gustafson-Barsis law, weak scaling:

$$Speedup = s + N * (1 - s)$$

Parallel Programming: types of parallel computing models



- Data parallel - the same instructions are carried out simultaneously on multiple data items (SIMD)
- Task parallel - different instructions on different data (MIMD)
- MIMD: Message passing (MPI) - overlapping computation and communication (!) , MATLAB Distributed Computing Server with Parallel Computing Toolbox
- SIMD: Array Programming (implicit parallelization), NumPy, High Performance Fortran, Vectorization (and **Tensorization**) in Matlab
- Task/data parallel paradigms : OpenMP, Fortran 2008 DO CONCURRENT
- Hybrid Programming: CPU-GPU, Intel Phi MIC architecture, SIMD$\rightarrow$OpenMP$\rightarrow$MPI

Parallel Programming: MPI in 5 minutes, task parallelism

Dynamic programming: value function iterations, heterogeneous types mapped to multiple processors

```
use mpi
integer :: nproc,id,ierr,sndr ! MPI
integer, dimension(MPI_STATUS_SIZE) :: STATUS ! MPI
! initializing MPI
 call MPI_INIT(ierr)
 call MPI_COMM_SIZE(MPI_COMM_WORLD,nproc,ierr)
 call MPI_COMM_RANK(MPI_COMM_WORLD,id,ierr)

  do i=n,1,-1 ! state space
      <compute V(i,t,id+1)>
  enddo ! state space
  call MPI_BARRIER(MPI_COMM_WORLD,ierr)
  do i=1,nproc-1
    if (id .eq. i) then
      call MPI_SEND(V,n,MPI_DOUBLE_PRECISION,0,id,MPI_COMM_WORLD,ierr)
    end if ! id > 0
...
    if(id .eq. 0) then
      call MPI_RECV(V,n,MPI_DOUBLE_PRECISION,MPI_ANY_SOURCE,MPI_ANY_TAG,
            MPI_COMM_WORLD,STATUS,ierr)
      sndr=STATUS(MPI_SOURCE)
      VV(1:n,t,sndr+1)=V
    end if !
    call MPI_BARRIER(MPI_COMM_WORLD,ierr)
  enddo ! i
call MPI_FINALIZE(ierr)
```

Tensors and Tensorization: implicit parallelization

- What is a tensor?
  - Tensor is an element of tensor space
  - Tensor space is a new vector space $\mathcal{W}$ constructed from components of vector spaces, for exampe, given $\mathcal{V}_1$ and $\mathcal{V}_2$: order two tensor $\mathcal{W} = \mathcal{V}_1 \otimes \mathcal{V}_2$
- Is a tensor a kind of vector? - Yes
- Is a matrix a special kind of tensor? - Yes and No
- With tensorization technique, multidimensional (multivariate) computations (linear programming, dynamic programming, MLE, likelihood ratio statistics) are much faster and more transparent than the corresponding single-dimension (univariate) computations

Hypercubes and hyperspheres:

tensorization and non-cartesian (adaptive, sparse) grids

- tensorization: robust, simple, stable, highly efficient, easily parallelizable brute-force attack
- human desire for more photo and video drives engineers to manufacture more efficient processors
- SIMD: common in modern processors in order to improve the performance of multimedia use (large number of vectors, data frames)
- GPUs and MICs are coming

Computing Moral Hazard Programs: SIMD and Tensorization

- Discretization: $\mathcal{C}$, $\mathcal{Q}$ and $\mathcal{A}$ are finite **ordered** sets.
- Key idea: build up multidimensional tensor object from low-dimensional vector objects while keeping the tensor structure in one-dimensional vector projection, then apply math operations to vectorized tensors
- Tensor product $\mathcal{C} \otimes \mathcal{Q} \otimes \mathcal{A}$
- MATLAB Kronecker tensor product: $KRON(X, Y) = X \otimes Y$

```
grc = linspace(0,4,41); %consumption
grq = [1 4];%output
gra = [0 .2 .4 .6 .8 1]; %action
nc = length(grc);nq = length(grq);na = length(gra);


%dimension of lottery vector per type
N = na*nq*nc;

C = kron(ones(1,na*nq),grc);
Q = kron(kron(ones(1,na),grq),ones(1,nc));
A = kron(gra,ones(1,nc*nq));

%participation constraints
b_neq = -U_0;
A_neq =  -u(C,A);

%objective function
Obj = Q-C;
```

Parallel Linear Algebra: ScaLAPACK and PETSc

ScaLAPACK:

- extends the LAPACK library to MIMD with distributed memory
- Language : Fortran, interfaces: C, C++, Fortran
- Dense systems
- Support in Commercial Packages: MKL - Intel, IMSL

PETSc:

- Portable Extensible Toolkit for Scientific Computation
- Scalable (parallel) solution of linear and non-linear PDEs
- Sparse systems
- Uses MPI for all parallel communications
- Distributed arrays
- Parallel Krylov subspace methods
- Parallel preconditioners
- Parallel (Newton-based) nonlinear solvers

GPU: OpenACC vs CUDA and OpenCL

- CUDA and OpenCL - highly complex C/Fortran instructions
- OpenACC - directive based standard that provides hints to compiler for a section of code to be offloaded from a host CPU to an attached accelerator.
- OpenMP (fully independent threads) → OpenACC (data dependent)

```
subroutine saxpy(n, a, x, y)
real(8) :: x(:), y(:), a
integer :: n, i

!OpenMP directive
!$omp parallel do
!OpenACC directive
!$acc kernels
do i=1,n
y(i) = a*x(i)+y(i)
enddo
!$acc end kernels
!$ omp end parallel do
end subroutine saxpy
...
$ main program
$ call SAXPY on 1M elements
call saxpy(2**20, 2.0, data_x, data_y)
```

MAGMA:

- "the number of cores will continue to escalate because of the desire to pack more and more components on a chip while avoiding the power wall, instruction level parallelism wall, and the memory wall"
- "there seems to be no doubt that future generations of computer systems, ranging from laptops to supercomputers, will consist of a composition of heterogeneous components"

M. Baboulin, J. Dongarra, J. Herrmann, and S. Tomov. "Accelerating linear system solutions using randomization techniques." ACM Transactions on Mathematical Software (TOMS) 39, no. 2 (2013)

New hybrid/fusion algorithms:

- Iterative MC (not to be confused with Monte Carlo simulations or integrations), main idea - construct **artificial random process** and to prove that the mathematical expectation of the process is equal to the unknown solution (or its functional) of the problem: "Monte Carlo Methods For Applied Scientists" by Ivan T. Dimov, 2005.
- K. Judd, L. Maliar and S. Maliar, (2012). "Merging Simulation and Projection Approaches to Solve High-Dimensional Problems".

Factors of computing performance:

from serial optimization to vectorization and parallelization

- Vectorization 7x by taking advantage of SIMD registers and SIMD instruction, strong scaling
- Parallelization on 16-cores, OpenMP multithreading 19x, weak scaling
- Phi co-processor, 244 threads, OpenMP multithreading 3.3x, weak scaling

Ninja gap: from pricing 4.7 Million options per second to pricing 12.3 Billion options per second

Shuo Li ,"Achieving Superior Performance on Black-Scholes Valuation Computing using Intel Xeon Phi Coprocessors", 2013

RCC at University of Chicago (Midway cluster)

ready to access high-performance computing for you

- 284 Shared Compute Nodes, 4544 Cores
- Each node has two eight-core 2.6GHz Intel Xeon E5-2670 "Sandy Bridge" processors with 32GB of main memory
- GPU Computing (GPU), 2 Tesla K20 devices per node
- MIC nodes, 2 Intel Phi devices per node
- Shared-Memory (SM), with 1TB main memory
- R, Python, MATLAB, STATA, IPOPT, Armadillo, Intel MKL, Intel MPI, Intel C++ and Fortran compilers, Portland C++ and Fortran

```
#!/bin/bash

#SBATCH --job-name=test_job
#SBATCH --output=test.out
#SBATCH --error=test.err
#SBATCH --nodes=1-1 --cpus-per-task=12
#SBATCH --time=1-12:00:00
module load matlab intelmpi
matlab -nodisplay -r "test"

sbatch test.batch
salloc --exclusive -n1 srun -n1 -N1 --pty --preserve-env $SHELL
scontrol show node  midway-g19-01
NodeName=midway-g19-01 Arch=x86_64  CoresPerSocket=8
    CPUAlloc=16 CPUErr=0 CPUTot=16 CPULoad=15.97  Features=lc,e5-2670,32G,noib
    OS=Linux  RealMemory=32000  AllocMem=32000  Sockets=2  Boards=1
```

Large-scale high performance computing resources

- DOE Oak Ridge Titan and TACC Stampede, open to researchers through the U.S. DOE INCITE program and NSF XSEDE program
- Number 2 and number 6 on `top500.org` list of the world's top supercomputers
- 560K cores, 710 terabytes of RAM, 8,209 kW (Titan); 462K cores, 192 terabytes of RAM, 4,510 kW (Stampede)
- Titan: 16C AMD Opteron CPUs, 2.2GHz and NVIDIA Tesla K20 GPU; Stampede : PowerEdge C8220, Xeon E5-2680 8C 2.700GHz, Intel Xeon Phi
- 27 Peta(10^{15})FLOPS (Titan), 8.5 PetaFLOPS (Stampede) (your PC $\approx$ 5-20 Giga(10^9)FLOPS)
- bitcoin network: $\approx$ 51 exaFLOPS (Nov 12, 2013)