

I D E A FUSION

Research and Education in Accelerator Physics at Old Dominion University

Balša Terzić, PhD

Department of Physics, Old Dominion University Center for Accelerator Science, Old Dominion University

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Accelerator Physics at ODU

Outline

- Accelerator Physics Education at Old Dominion University
 - Center for Accelerator Science (CAS)
 - Research Experience for Undergraduates (REU) at ODU
- Accelerator Physics Research at Old Dominion University
 - Research directions within CAS
 - Computational accelerator physics
 - Outline a few projects
 - Optimization using Genetic Algorithms
 - Computation on Graphical Processing Units (GPUs)
- Summary

Accelerator Physics Education at ODU

- Interdisciplinary Center for Accelerator Science (CAS) at ODU (<u>http://www.odu.edu/cas</u>)
 - Founded in 2008 as an umbrella center for interdisciplinary approach to solving accelerator physics problems (note "Science" not only "Physics")
 - Members from several departments
 - Physics (6 professors), computer science (2), engineering...
 - Capitalizes on the proximity of Jefferson Lab
 - 3 Jefferson Lab Professors (Jefferson Lab staff; spend 30% of time at CAS)
 - Accelerator physics students carry out their research at Jefferson Lab
 - Current numbers:
 - 13 graduate students
 - 2 postdocs
 - Graduated 7 PhDs in physics and 3 PhDs in engineering

Accelerator Physics Education at ODU

- Research Experience for Undergraduates (REU) at ODU (<u>https://www.jlab.org/accel/reu/</u>)
 - Highly selective, NSF-sponsored, 10-week paid summer program
 - Starts at the end of May, ends at the end of July
 - Students are housed on Jefferson Lab's campus
 - Weekly lectures on various research topics
 - Guidance provided on scientific writing and presentation
 - Many, free "mandatory fun" events are planned
 - Students are supervised by ODU professors or Jefferson Lab staff
 - At the end, students write a research paper and present posters
 - They are often chosen to present their work at national conferences
 - Current numbers (since 2008):
 - 53 students (15 female); 32 did research in accelerator physics

Accelerator Physics Education at ODU

- Summer Undergraduate Laboratory Internship (SULI) at Jefferson Lab (<u>http://education.jlab.org/suli/</u>)
 - Highly selective, DoE-sponsored, 10-week paid summer program
 - Starts at the end of May, ends at the end of July
 - Students are housed on Jefferson Lab's campus
 - Weekly lectures on various research topics
 - Guidance provided on scientific writing and presentation
 - Many, free "mandatory fun" events are planned
 - Virtually identical to REU, but only Jefferson Lab staff and users can serve as student mentors
 - Not a problem: virtually all of ODU physics professors are either Jefferson Lab staff or users (all of CAS members)
 - At the end, students write a research paper and present posters
 - They are often chosen to present their work at national conferences

Accelerator Physics Research at ODU

- Detailed description of accelerator research projects: <u>http://www.odu.edu/cas</u>
- Superconducting radio-frequency (SRF) accelerating structures (Professor Jean Delayen, CAS Director)
- Novel materials for future superconducting cavities (Professor Alex Gurevich)
- Plasma processing of superconducting structures (Professors Vušković and Popović)
- Accelerator design: Energy-recovering linacs, electron-ion colliders, light sources, energy-recovering linacs (Professors Krafft, Satogata,...)
- And others...

My Accelerator Physics Research at ODU

- New computational tools:
 - New methods
 - New computational hardware
- New methods: Multidimensional, nonlinear optimization using genetic algorithms (GA)
 - Brief motivation and background
 - Applications in accelerator physics
- New computational hardware: Parallel computation on Graphical Processing Units (GPUs)
 - Brief motivation and background
 - Applications in accelerator physics

Why Computations?

- Any scientific field can benefit from computations
 - Experimental sciences: data processing, model validation
 - Theoretical sciences: simulate physical processes, model validation
 - *Discovery science*: e.g. Lorenz's (re-)discovery of chaos in 1970's
- New computer architectures resolve old computational bottlenecks
 - Present state-of-the-art unfathomable even 5-10 years ago:
 - Codes now can utilize on the order of *millions of processors*
 - Particle simulations: 1 simulation particle = 1 electron in a bunch
 - Relax approximations/simplifications \rightarrow closer to the physics problem
 - What once was computationally prohibitive it is now possible
- Accelerator physics critically relies on computations for
 - Validate new concepts: no study without it is taken seriously
 - Performance optimization

Computations in Accelerator Science

- Prodigious increase in computational power
 - → Relaxing simplifying approximations (i.e., $1D \rightarrow 2D \rightarrow 3D$)
 - \rightarrow More trustworthy computer simulations
- Cannot be a "one-trick pony"
 - State-of-the-art computations require *all of these*:
 - Fundamental understanding of underlying physics
 - Utilization of (new) advanced mathematical techniques
 - Computational expertise (including newest computational platforms)
- Computations in accelerator science *must be interdisciplinary*
 - Utilize field experts in physics, computer science, math, engineering...
 - Center for Accelerator Science (CAS) proposal (2007), 1st paragraph:

"We propose an interdisciplinary research and teaching center for accelerator science and technology. It would be unique in Virginia and one of only a handful of such programs in the country. Since <u>accelerator science is inherently interdisciplinary</u>, the center would be a source of innovation in pure and applied science, which is likely to engender spin-off industry and add to the university's capacity for generating patents."

GA Optimization: Motivation

- Multidimensional non-linear optimization becomes more challenging/ impossible as the dimensionality of the problem increases
 - Traditional, gradient-based methods (Newton, conjugate-gradient, steepest descent, etc...) are <u>not globally convergent</u>:
 - May get stuck in a local minimum and never come out
 - Final solution depends on the initial guess
 - Generally *not robust* in the non-linear regime
 - Direct multi-objective optimization not possible
- This demonstrates a clear need for *globally-convergent, robust, multidimensional, multi-objective, non-linear optimization* methods
 - Genetic Algorithm (GA) fills this need
 - Trade-off: not as efficient as traditional methods

GA Optimization: Background

• GA uses principles of natural selection to solve an optimization problem

| Evolution | Multidimensional optimization | | | |
|----------------|-----------------------------------------|--|--|--|
| Gene | Variable | | | |
| Individual | Point in search space | | | |
| Population | Set of points in search space | | | |
| Mutation | Changing variables | | | |
| Swap | Exchange of values of the same variable | | | |
| | between two points in search space | | | |
| Recombination | Change of values of the same variable | | | |
| (partial swap) | between two points toward each other | | | |
| Fitness | Value of the objective function | | | |

- Mutation
 - Similar to random walk Given by a pdf $P_m(\eta_{mut})$
- Recombination
 - Given by a pdf $P_r(\eta_{rec})$

 $\eta_{mut}=1$ $\eta_{mut}=10$ $\eta_{rec}=1$ $\eta_{rec}=10$

[Hofler, Terzić, Kramer, Zvezdin, Morozov, Roblin, Lin & Jarvis 2013, Phys. Rev. ST AB 16, 010101]

Accelerator Physics at ODU

Students' names underlined

GA Optimization: Background



2 April 2015

Accelerator Physics at ODU

GA Optimization: Applications

We applied GA optimization to many problems in accelerator physics:

- Beam diagnostics (wire scanner fits) [REU Projects: Henderson 2013, Gabriele 2014] objective Optimizing particle collider working point for luminosity Maximizing dynamic aperture in a particle collider ring Decoupling of the beam optics in the injector Multiple
 - Optimizing dynamic aperture and chromaticity in a collider ring
 - RF gun optimization for injector brightness [Hofler, Terzić, Kramer, Zvezdin, Morozov, Roblin, Lin & Jarvis 2013, Phys. Rev. ST AB 16, 010101]
 - Optimizing laser frequency modulation function in Thomson scattering [Terzić, Deitrick, Hofler & Krafft 2014, Phys. Rev. Lett., 112, 074801]
 - Optimizing cavity heat load and trip rates in CEBAF linacs at Jefferson Lab [Terzić, Hofler, Reeves, Khan, Krafft, Benesch, Freyberger & Ranjan 2014, Phys. Rev. ST AB 17, 101003]
 - Real applications for real machines
 - CEBAF and the proposed Medium-energy Electron Ion Collider (MEIC) at Jefferson Lab, but not limited to these

Single

objectives

GA Application: Optimizing Cavity Heat Load and Trip Rates in the CEBAF Linacs

- What is the optimal configuration of cavity gradients needed to maximize the science and minimize the cost of operation (electricity bill)?
 - Monthly electricity bill for JLab is measured in millions of dollars

 a large part of it is CEBAF cryogenics
 Even modest improvements in cooling may translate into millions in savings
 - Cooling (cavity heat load) and interrupted operation time (trip rates) are *competing objectives* – multi-objective optimization problem
- The goal here:
 - Provide a set of feasible solutions showing the *trade-offs between* competing objectives
- Asymptotic behavior provided by 1D minimization using Lagrange multipliers

[Terzić, Hofler, <u>Reeves</u>, <u>Khan</u>, Krafft, Benesch, Freyberger & Ranjan 2014, *Phys. Rev. ST AB* 17, 101003]



GA Application: Optimizing Cavity Heat Load and Trip Rates in the CEBAF Linacs



(4% from the minimum of 1048 W @ A)

Reduced heat load by 15%

(Savings exceed my salary many times over!)

[Terzić, Hofler, <u>Reeves</u>, <u>Khan</u>, Krafft, Benesch, Freyberger & Ranjan 2014, *Phys. Rev. ST AB* 17, 101003]

GA Application: Narrow-Band Emission in Thomson Scattering



[Terzić, Deitrick, Hofler & Krafft 2014, Phys. Rev. Lett., Phys. Rev. Lett., 112, 074801, Fig. 1]

- Thomson scattering:
 - Classical regime: no electron recoil, no quantum effects
 - Factor of $4\gamma^2$ increase in energy

 $E_{\rm radiation} = \gamma^2 (1+\beta)^2 E_{\rm laser} \approx 4\gamma^2 E_{\rm laser}$

- Constant-frequency laser produces *broadened spectra* in high-field regime [Krafft 2004, *Phys. Rev. Lett.* 92, 204802]
- Can a judicious laser frequency modulation ("chirp") lead to narrowing of the spectra? We believed so.
- $\mathbf{Scaled Frequency}$ [Krafft 2004, Fig. 2] low field high field

• Enter GAs

GA Application: Narrow-Band Emission in Thomson Scattering

- After some heuristic investigation (*educated guessing!*), we settled on a two-parameter modulation function: $f_{GA}(\bar{\xi}; b, c) = c/\left[1 (1 c)\exp\left(-b\bar{\xi}^2\right)\right]$
- We set up a GA optimization which
 - Maximize the height of the main peak
 - Minimize the width at 10⁻⁶



GA optimization provided vital clues about the shape of the modulation function which was later found exactly and analytically [Terzić, <u>Deitrick</u>, Hofler & Krafft 2014, *Phys. Rev. Lett.*, *Phys. Rev. Lett.*, 112, 074801]



GPU Computation

- Why is it important?
 - Making simulations much more efficient computationally (through GPUs) enables studying previously inaccessible physics
- What are we doing that is new and different?
 - Interdisciplinary approach division of labor among experts in the field:
 - Physicists: physics, algorithm development, prototyping
 - Computer scientists: algorithm development and implementation, parallel programming
- What are our goals?
 - Develop GPU-parallelized *state-of-the-art accelerator physics codes*
 - Design methods useful *beyond the scope of accelerator physics*
 - Develop expertise useful on other problems and other architectures

GPU Computation: Motivation

- There are many problems in accelerator physics that can greatly benefit from a speedup from a GPU-based computation
 - Particle tracking codes
 - Beam collision codes
 - Monte Carlo-based codes
- *Speedup*: ratio of execution times on a host CPU to that on a GPU
- Some have already been GPU-parallelized with impressive speedup of about 20 70 times
- In general, if a problem is inherently parallelizable, an implementation on GPUs can improve performance by 1-3 orders of magnitude
- This kind of speedup means:
 - Simulation time: several months or a year \rightarrow about a day
 - Opening the doors to studying previously inaccessible physics!

GPU Computation: Background

- Parallel computation on GPUs
 - Ideally suited for algorithms with *high arithmetic operation/memory access ratio*
 - Same Instruction Multiple Data (SIMD)
 - Several types of memories with varying access times (global, shared, registers)
 - Uses extension to existing programming languages to handle new architecture
 - GPUs have many smaller cores (~400-2500) designed for parallel execution
 - Avoid branching and communication between computational threads



GPU-Based Simulations of Electron Beams

- Physical Problem
 - When electron beams are bent, they radiate
 - The radiation "catches up" and adversely affects the beam (breaks it up and renders useless)
 - Numerical simulation difficult and computationally prohibitive because of integration over beam's history
- Importance
 - Dynamics of electrons in most electron machines
 - Better simulations lead to better understanding of electron beam's dynamics and mitigation of the unwanted effects

Our contribution

- Designed a new adaptive multidimensional integration algorithm optimized for GPUs [<u>Arumugam</u>, Godunov, Ranjan, Terzić & Zubair 2013a, b]
 - Useful beyond this project
- Achieved over 3 orders of magnitude speedup over a serial code [Terzić, <u>Arumugam</u>, Godunov, Ranjan & Zubair 2015, Phys. Rev. ST AB, *in preparation*]

Summary

- Strong accelerator physics educational program at ODU
 - CAS, REU, SULI @ Jefferson Lab
 - Students involved in cutting-edge research
 - Publish, go to conferences in exotic locations, graduate, get good jobs!
- Computational Accelerator Physics Research at ODU
 - Interdisciplinary collaboration at CAS
 - High-performance computations
 - Using GAs to optimize performance and design of accelerators
 - Parallel computations on GPUs
- We are always on a lookout for hard-working, motivated students, so if you are interested, please get in touch!

More info: <u>http://www.odu.edu/cas</u> <u>http://www.odu.edu/~bterzic</u> <u>bterzic@odu.edu</u> <u>http://www.odu.edu/~bterzic</u>

My Interdisciplinary Collaborators

Center for Accelerator Science (CAS) at Old Dominion University (ODU): Professors:

Physics: Alexander Godunov

Computer Science: Mohammad Zubair, Desh Ranjan

PhD students:

Physics: Kirsten Deitrick

Computer Science: Kamesh Arumugam, Sabbir Khan, Mohamed Aturban

Undergraduate students:

Physics: Mark Stefani, Marvin Munoz

Jefferson Lab (Newport News):

Accelerator Division:

Geoff Krafft, Alicia Hofler, Vasiliy Morozov, Fanglei Lin, He Zhang, Yves Roblin, Jay Benesch, Arne Freyberger

Nuclear Theory Group:

Wally Melnitchouk

Undergraduate Summer Interns (REU and SULI programs) (7 since 2010)

Colin Jarvis, Matt Kramer, Anton Zolotor, Alyssa Henderson, Cody Reeves, Victoria Gabriele, Todd Hodges

Details at http://www.odu.edu/~bterzic

Refereed Publications:

- Terzić, Deitrick, Hofler & Krafft 2014, Phys. Rev. Lett., 112, 074801
- Terzić, Hofler, <u>Reeves</u>, <u>Khan</u>, Krafft, Benesch, Freyberger & Ranjan 2013, *Phys. Rev. ST AB* 16, 010101
- Hofler, Terzić, Kramer, Zvezdin, Morozov, Roblin, Lin & Jarvis 2013, Phys. Rev. ST AB 16, 010101
- <u>Arumugam</u>, Godunov, Ranjan, Terzić & Zubair 2013a, International Conference on Parallel Processing – 42nd Annual Conference (refereed)
- <u>Arumugam</u>, Godunov, Ranjan, Terzić & Zubair 2013b, 20th Annual International Conference on High-Performance Computing (refereed)
- Terzić & Bassi 2011, Phys. Rev. ST AB 14, 070701

Conference and Other Contributions:

- Arumugam, Godunov, Ranjan, Terzić & Zubair 2013, GPU Tech conference
- Henderson, Terzić & Hofler 2013, REU (@ODU) project
- Roblin, Morozov, Terzić, <u>Aturban</u>, Ranjan & Zubair 2013, International Particle Accelerator Conference (MOPWO080)
- Terzić, <u>Kramer & Jarvis</u> 2011, Particle Accelerator Conference (WEP167)
- Kramer, Jarvis & Terzić 2010, JLab Tech Note JLAB-TN-10-034

Backup Slides

GPU-Based Particle Collider Simulations

• Physical Problem

- Simulate long-term behavior of colliding beams in a collider
- Colliding beams disturb each other slightly during each collision
- One hour of collider operation is on the order of billion collisions!
- New, efficient algorithms and architectures are needed
- Importance
 - Dynamics of electrons in most electron machines
 - Better simulations lead to better understanding of collider's long-term dynamics and mitigation of the unwanted (resonant) effects

Our contribution

- Designed a new GPU-optimized particle tracking algorithm [Arumugam, Godunov, Ranjan, Terzić & Zubair 2015, *in preparation*]
 - Useful beyond this project
- Implementing a tracking + collision code [Terzić et al. 2015, Phys. Rev. ST AB, *in preparation*]

Tomography

- Physical Problem
 - Recover 2D/3D shape from a set of 1D projections
- Importance and Applications
 - Accelerator physics (beam diagnostics)
 - Plasma physics, medical physics, astrophysics
- What Needs to Be Done



- Effects of noise in experiments (noise removal wavelets)
- Quantify the accuracy of reconstructed image vs. number of projections
- Student Skills Developed
 - Mathematical physics (integral equations, integration methods...)
 - Computational physics (all work is done on computers)

Wavelet Denoising and Compression



Wavelet denoising yields a representation which is:

- Appreciably more accurate than non-denoised representation
- Sparse (if clever, we can translate this sparsity into computational efficiency)

Parallel Computation on GPUs

- The largest resolution tested so far is 128x128
- 1 step of the simulation on a 128x128 grid and 32 GPUs: ~ 10 s
- Execution time *reduces* as the number of macropraticles grows

| Number of | Grid | Sequential | Single GPU | | 32 GPUs | |
|---------------|------------------|------------|-------------|---------|-------------|---------|
| Particles (N) | Resolution | Time(sec.) | Time (sec.) | Speedup | Time (sec.) | Speedup |
| 102400 | 32×32 | 145.52 | 1.48 | 98 | 1.29 | 113 |
| | 64×64 | 1736.24 | 16.78 | 104 | 1.13 | 1537 |
| | 128×128 | 27049.30 | 256.85 | 105 | 13.88 | 1950 |
| 1024000 | 32×32 | 121.41 | 1.30 | 93 | 1.23 | 99 |
| | 64×64 | 1140.15 | 11.12 | 103 | 1.75 | 652 |
| | 128×128 | 15153.60 | 144.03 | 105 | 11.78 | 1287 |
| 4096000 | 32×32 | 119.73 | 1.29 | 93 | 1.23 | 97 |
| | 64×64 | 939.96 | 9.19 | 102 | 1.74 | 540 |
| | 128×128 | 10654.00 | 101.37 | 105 | 9.33 | 1142 |

GPU Computation: CSR Simulations



- CSR adversely impact beam quality:
 - Increased energy spread and emittance, longitudinal instability (microbunching)
- CSR effects are important for machines which bend electrons (FELs, light sources, ERLs, electron colliders, etc...)
 - JLab FEL, LCLS-II, NSLS-II, ALS, Fermi@ELETTRA...
- It is of vital importance to have a trustworthy code to simulate and mitigate the CSR effects

GPU Computation: CSR Simulations

- CSR simulations have proven to be extremely challenging
 - Computing *retarded potentials* requires integration over the retarded time t':

$$t' = t - \frac{\left|\vec{r} - \vec{r}'\right|}{c} \qquad \left[\begin{array}{c} \phi(\vec{r}, t) \\ \vec{A}(\vec{r}, t) \end{array}\right] = \int \left[\begin{array}{c} \rho(\vec{r}', t') \\ \vec{J}(\vec{r}', t') \end{array}\right] \frac{d\vec{r}'}{\left|\vec{r} - \vec{r}'\right|} \qquad \left(\begin{array}{c} \phi(\vec{r}, t) \\ t_{0} \\ t_{1} \\ t_{2} \end{array}\right)$$

Retarded time

Retarded potentials

Charge & current distribution

- Huge computational bottleneck!
- For a particle-in-cell (PIC) CSR code the computations scale as ~ N_{res}² (N_{res} is the grid resolution)
- Solution: Develop an efficient, parallel multidimensional integrator on GPUs
 - Integration over grid is ideally suited for GPU parallelization (SIMD)
 - Used NVIDIA CUDA framework (extension to C++)
 - *Deterministic*: based on integration rules like Gauss or Newton not Monte Carlo
 - Useful beyond this project: *outperforms Monte Carlo in medium/high dimensions*

Circles of

causality

Adaptive Multidimensional Integration On a Single GPUs

- Direct parallelization of the serial methods *does not take advantage of GPU data* parallelism and *does not provide load balancing* → *inefficient code*
- We developed a new two-phase parallel algorithm multidimensional integration on GPUs
 - Phase 1: Parallel identification of subintervals needing higher resolution
 - Phase 2: Parallel evaluation of identified sub-regions to prescribed accuracy
- GPU-based implementation outperforms the best known sequential method (CUHRE) and achieve up to 10-100 times speedup on a single GPU



[Arumugam, Godunov, Ranjan, Terzić & Zubair 2013a]

Adaptive Multidimensional Integration On Multiple GPUs

- Next, we *optimized* our new GPU-based algorithm *for memory efficiency* and ٠ scaled to multiple GPU devices
- The algorithm has been implemented on a cluster of Intel[®] Xeon[®] CPU X5650 ٠ computes nodes with 4 Tesla M2090 GPU devices per node (512 cores per device)
- Memory optimization on a single GPU earned us another factor of 3.5 ٠ (speedup increased from 70 to 240)
- Scaling up to 24 GPU devices earned us another factor of 13.5 ٠ (speedup increased from 240 to 3250)



[Arumugam, Godunov, Ranjan, Terzić & Zubair 2013a, 2013b]

24

f2(x) +

Monte Carlo Vs. Adaptive Multidimensional Integration With a Single GPU

- Monte Carlo integration on GPU (VEGAS and BASES methods) has been published previously in *The European Physical Journal C* [Kanazaki 2011, 71:1559]
- We compare Monte Carlo Vs. our method on a set of 6 functions with exact solutions
- *Preliminary results*: Even in higher dimensions our adaptive multidimensional integration method outperforms Monte Carlo method on a single GPU
- *Preliminary results*: Monte Carlo on GPU fails for large number of function evaluations
- Possible ramifications: Our new code can replace Monte Carlo in many physics application for improved performance



[Arumugam, Godunov, Ranjan, Terzić & Zubair 2014]

GA Application: Optimizing Collider Working Point

- As particles circulate in collider rings, they oscillate around design orbits in both *x* and *y* transverse directions: *betatron oscillations*
- Collider luminosity is sensitive to beam-beam effect and betatron resonances of the two colliding beams
- Careful selection of a tune *working point* is essential for stable operation of a collider as well as for achieving high luminosity
- Simulate the proposed Medium-energy Electron-Ion Collider (MEIC) at JLab
- *Optimization problem*:
 - Independent variables: betatron tunes for the two beams $(v_{x}^{1}, v_{y}^{1}, v_{x}^{2}, v_{y}^{2})$
 - Objective function: collider's luminosity $L(v_x^1, v_y^1, v_x^2, v_y^2)$ (Evaluated via a simulation with *BeamBeam3D* parallel code on the JLab cluster)
 - Subject to constraints (e.g., confine tunes to particular regions)
- GA is the only non-linear optimization method that can work in a search space so violently fraught with resonances (*very* sharp peaks and valleys)

GA Application: Optimizing Collider Working Point

- Resonances occur when $m_x v_x + m_y v_y = n$ m_x , m_y , and n are integers
- Green lines: *difference* resonances (stable)
- Black lines: *sum* resonances (unstable)
- Restrict search to a group of small regions along the diagonal devoid of black resonance lines. Restricts the search space by ~30 in 2D, ~1000 in 4D
- Found an excellent working point near half-integer resonance

e-beam: $v_x = 0.530$, $v_y = 0.548$ p-beam: $v_x = 0.501$, $v_y = 0.527$

- Luminosity about 33% above design value in only ~300 simulations (5 gen. of 64 individuals)
- Systematic scan with a modest 0.01 resolution: 100⁴=10⁸ simulations!

➔ GA search orders of magnitude more efficient

• This is just a proof of principle – future realistic simulations will include other important effects: magnet errors, non-linear maps, IBS, cooling ...

