

James D. Freels

COMSOL-Related Activities within the Research Reactors Division of Oak Ridge National Laboratory

Abstract Our group at Oak Ridge National Laboratory (ORNL) started using COMSOL shortly after version 3.0 was released in the Spring of 2004. Over 11 years later and several new releases of the code, the application usage has grown along with the number of licenses we are responsible for. This paper focuses not on details of results and modeling methods, but instead, takes a look at our past and present applications, and evaluates where we are headed with COMSOL in the future. In doing so, we reveal some lessons learned along our pathway, provide some insight on how best to use COMSOL in a group setting, and perhaps help both users and developers to improve how the code is utilized.

1 Introduction

Early in my career as an engineering analyst in the nuclear industry, my perception was that we probably analyzed systems, structures, and components to a greater extent than other industries. As such, I preformed many numerical simulations using legacy codes, or codes that we wrote ourselves to perform the task at hand. We would often state, “there has to be a better way to do this.” It seemed that the codes were so slow, limited in their application, and prone to problems with stability and accuracy. Indeed, this was one motivation for pursuing further study; that is, I wanted to really find out what was available beyond what I was currently exposed to.

Fortunately, excellent mentoring was provided, both from my work and academic environments. This eventually led me to realize that concepts such as finite-element methods, fully-implicit time stepping, parallel processing, etc., were available. In turn, this led me to decide what type of code would be worth spending resources upon, especially my own time.

Oak Ridge National Laboratory
1 Bethel Valley Road
P.O. Box 2008
Oak Ridge, TN 37831-6392
Office: (865)576-8645
Fax: (865)241-2712
E-mail: freelsjd@ornl.gov

Upon my start at ORNL, one primary goal, was to demonstrate and pass on to the next generation of nuclear engineers, these methods that I believed to be the best choice. Specifically, I wanted to utilize the Research Reactors Division (RRD) and the High Flux Isotope Reactor (HFIR) to reach this goal since it seemed that the best opportunity would be at one of the world’s best research reactors at ORNL.

2 Why We are Using COMSOL

After several years of looking for the right code that met my criteria, including a few mistakes and bad investments along the way, it is pleasing to have available a code such as COMSOL to perform our engineering analysis work. It is a good idea to occasionally review what these criteria are, and make sure that the code choice is still valid. Hence, I will attempt to summarize the main reasons for choosing COMSOL.

My one sentence description of COMSOL is a “finite-element based computer simulation toolbox.” My colleague, Dr. Prashant Jain, who obviously continues to be pleased that I introduced him to COMSOL, describes it differently. Prashant’s one-sentence for COMSOL is “the SmartPhone of Multiphysics.” Indeed Prashant has developed a separate presentation he calls the “25 Must-Have ‘User-Centric’ Features for any Engineering Analysis Software” that I would encourage you to examine. Therefore, the reasons for using COMSOL can be different for different people, and please don’t think that my reasons are valid for all people.

My COMSOL choice is based as follows:

- Finite-element methods are the most accurate numerical simulation tool available for deterministic solutions. This can be a controversial statement to some people, and I hope I do not offend anyone by saying this. My studies have proven this out, and shown this to be true from my experiences.[1]
- COMSOL is essentially a 100% -true finite-element method code for all the physics simulated (some exceptions: ODE solver, Particle Tracing Module). One of the first things I did when starting with COMSOL is

to confirm the expected convergence rate of the solution error with mesh refinement as a function of finite-element interpolate order (linear, quadratic, cubic, etc. with a mouse click).[2]

- COMSOL is the leader, and perhaps, the only true-multiphysics code commercially available (CFD, heat transfer, structural mechanics, PDE mode, etc. on our projects) that I have been able to find. This is also subject to debate, and could change with time.
- If desired, the standard equations solved may be altered on INPUT by the USER (for example, constitutive equations including turbulence model). This feature alone removes the need to “write your own code.”
- You can solve your own equations from scratch (PDE, ODE, algebraic, functions, etc.). It is no longer necessary to write complex, error-prone, lines of source code. I tend to think of COMSOL as a higher-level language; a different way of writing code.
- COMSOL provides a convenient GUI in modern computing environments. There is a lot of discussion about the many nice features of the COMSOL GUI in Prashant’s “25 Must-Have User-Centric” list.
- COMSOL continues to provide technical support and code improvements at a remarkable pace (distributed parallel processing, new modules, interface tools, response to user requests, etc.) and is now up to version 5.1. This is what the annual subscription fee for, but if you compare the development pace to other commercial codes, or other sponsored codes with a staff of developers, you will find COMSOL near the top while remaining at a high level of quality.
- The new “Application Builder” is now available with the base package. We have not used this feature to a great extent, but we have found some valuable features inside this part of the code package (for example, an integrated java editor).

3 Some Success Stories

We have used COMSOL on several applications, but there are two primary success stories that I will highlight here. The first is a key component in our hydrogen cold source[3, 4,5] called the hydrogen loop pressurizer, or pressurizer. This component provides the main interface between the outside (ambient) environment and the pressurized cryogenic hydrogen loop that includes the cold source moderator vessel. An as-built view, before all the insulation is applied, is shown in Fig.1.

COMSOL Multiphysics played a key role in the design of this component. In particular, the code was used to determine the heat transfer and natural convection of the cryogenic hydrogen within the component as depicted in Fig.2 and Fig.3, respectively. The primary goal of the analysis was to determine the proper placement of a copper strap alongside the lower vessel of the pressurizer which provides a critical mass of high-density hydrogen within

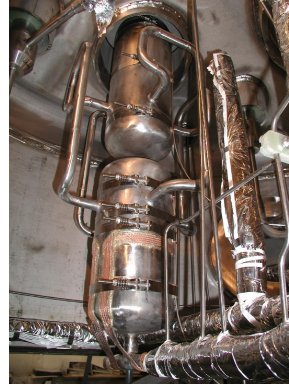


Fig. 1 As-Built View of the HFIR Hydrogen Cold Source Pressurizer

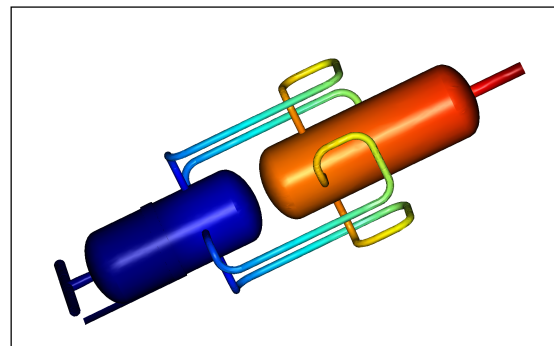


Fig. 2 COMSOL-Predicted HFIR Hydrogen Pressurizer Heat Conduction

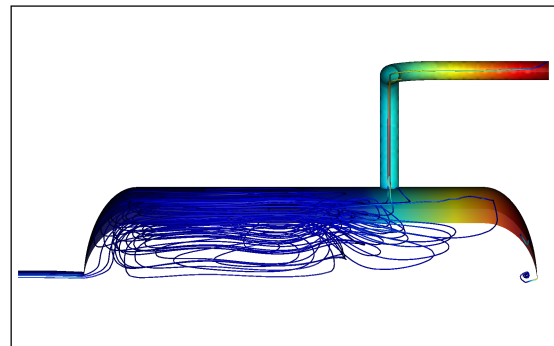


Fig. 3 COMSOL-Predicted HFIR Hydrogen Pressurizer Natural-Convection Fluid Flow

the lower part of the vessel; which eventually interfaces directly with the cryogenic loop.

The completed HFIR cold source has been in place for over 10 years and has provided cold neutrons for over 50 HFIR fuel cycles of operation.

Another success story has been the utilization of COMSOL for the development of a major new isotope production project at the HFIR.[6,7] HFIR is presently involved in a project to demonstrate the production of Pu-238 for

NASA to provide a fuel-source for deep-space travel of exploration vehicles such as the present Curiosity Mars rover.[8, 9]

The development program has been carried out in several stages with the earliest test irradiation performed on a “bare pellet” configuration as depicted by the COMSOL solution in Fig.4. Additional bare-pellet irradiation was performed, including a “reduced-length” pellet, in order to determine unknowns in the pellet properties. The initial irradiation was carried out using extremely conservative settings for the NpO_2 (used as the unirradiated material to produce the Pu-238 material upon irradiation) pellet material properties. The next stage in development was to

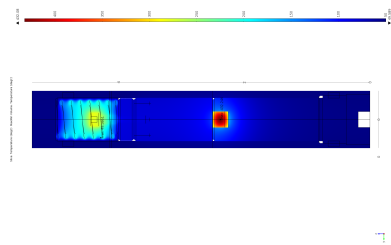


Fig. 4 COMSOL Cut-Plane Temperature Solution for 3D Simulation of the HFIR Pu-238 Demonstration Irradiation of the Bare-Pellet Design (shown rotated 90° from the true orientation, magnified viewing of .pdf file recommended to see the details)

insert a “partially-loaded” target into HFIR that was designed to demonstrate an increased loading. Depicted in Fig.5 as a COMSOL-predicted temperature surface, the 2D axisymmetric model allowed for seven pellets to be modeled based on the results from the bare-pellet models.

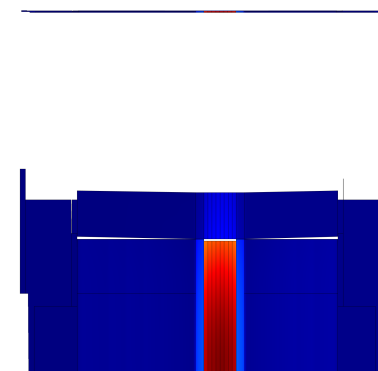


Fig. 5 COMSOL 2D Axisymmetric Temperature Solution for the Simulation of the HFIR Pu-238 Demonstration Irradiation of the Partially-Loaded Target Design (shown rotated 90° from the true orientation). Top-physical view to scale, Bottom-screen view not to scale.

Eventually, the project arrived at a “final” design. The design could still change as improvements in material property measurements from post-irradiation examination, COMSOL model details, and new innovations in the design, are obtained. The current design includes 52 pellets inserted into the target as depicted in Fig.6 as a temperature surface from the 2D axisymmetric COMSOL model.

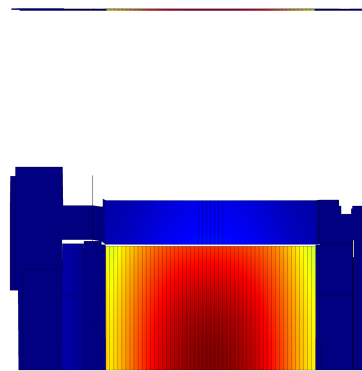


Fig. 6 COMSOL 2D Axisymmetric Temperature Solution for the Simulation of the HFIR Pu-238 Demonstration Irradiation of the Fully-Loaded Target Design (shown rotated 90° from the true orientation). Top-physical view to scale, Bottom-screen view not to scale.

The current COMSOL model of the Pu-238 development target includes the following physics: (a) heat conduction, (b) structural mechanics, (c) structural contact, (c) thermal expansion, (d) gas-gap conductance, (e) and pseudo-steady time dependence of all properties including fission-gas production during the HFIR fuel cycle. Each individual pellet is explicitly modeled as depicted in Fig.7. Complete structural contact is allowed between the pellet and target housing. The maximum temperature drop occurs across the gas gap containing a mixture of helium fill gas, and fission-product gases as they build during the HFIR irradiation cycle.

4 Our Current Applications

Our most active current project, with extensive use of COMSOL, is a research project investigating the conversion of the High-Flux Isotope Reactor (HFIR) of ORNL from high-enriched uranium (HEU) to low-enriched uranium (LEU) fuel. As the project has progressed in time, two major areas of model development have evolved: (1) a safety-basis (SB) model which utilizes the $k-\epsilon$ turbulence model with less mesh density and quicker turn-around time for solutions, and (2) a best-estimate (BE) model which utilizes the SST low-Reynolds turbulence model and results

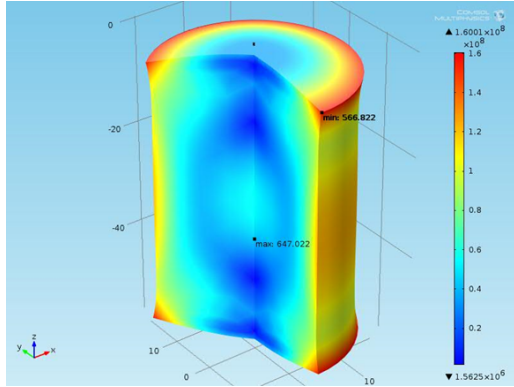


Fig. 7 An individual pellet at the maximum temperature within the pellet stack in the COMSOL 2D axisymmetric solution of a fully-loaded target (note: classic hourglass shape). This particular plot is shown as a 3-D rotated stress contour with 10000x deformation of the hot pellet at HFIR position VXF-15, the end of a single irradiation cycle, and safety-basis conditions of 130% Power.

in higher mesh density and computer resources. The SB model is initialized at conservative conditions, is designed to yield worst-case scenario results, and produces many of the traditional safety-related parametric results such as incipient boiling, flow excursion, and burn-out conditions. The BE model is designed with solution accuracy as a goal, such that a sufficiently refined mesh adjacent to the nuclear fuel-plate heated wall yields the best possible CFD solution available with COMSOL. Safety studies are still possible with the BE model, but primarily as sensitivity studies of single perturbations, rather than an “all-at-once” worst case as produced by the SB model. Both models compliment each other, and can be used to take advantage of the benefits of each to provide answers to specific questions about the analyzed LEU fuel design.

Several areas of research are ongoing whereby COMSOL modeling is expanding into our current base models. Separate-effects models have been developed for (a) isothermal fluid-structure interaction (FSI)[10,11], (b) hot-spot analysis via fuel segregation, and non-bonding[12], (c) temperature - dependent solid material properties[13], (d) pressure and temperature dependence of water properties based on NIST standards[14], and (e) thermal-structure interaction (TSI) caused by thermal expansion[15].

Time and space are limited in this paper in order to provide detailed discussion of the current results for this project here. The reader is encouraged to examine the cited references herein for these details.

5 Anticipated Expansion of our Applications

Additional separate effects models are also being developed for both the LEU conversion project and for generalized HFIR improvement including: (a) non-iso-thermal fully-coupled FSI, (b) additional irradiation impacts including fuel swelling, (c) multi-plate models up to and including the entire core, (d) reactor physics by diffusion

theory and discrete ordinates using equation-based modeling, (e) flow blockage, and (f) other severe accidents. Proof-of-concept developments have already been completed for items (a) through (d) inclusive. The reader should review past and current publications for more detailed information [16,17,18] including papers and posters submitted to the present conference.

6 Best Practices

As we increase our COMSOL usage and users, opportunities of a different sort present themselves that are more managerial and logistic than software related. This section provides some details on the following activities taking place at our facility that may be of interest to the readers of this paper: (1) software, license, and documentation management, (2) local COMSOL user group, (3) joint ORNL / COMSOL symposia / workshops, (4) local tips and tricks library, and (5) software quality assurance.

6.1 Software, License, and Document Management

During our initial trial license period in 2004, the COMSOL sales staff were very patient and allowed us to have a longer than normal trial period. This turned out to be a significant benefit for both parties. We really needed to clearly show a benefit for the software purchase for our management to see in order to gain approval for the purchase. While ORNL is certainly accustomed to purchasing software, this was a significant purchase, and COMSOL was not a routine purchase for ORNL at the time. In addition, by allowing us the extra trial-period, our group has since become a loyal customer, and several licenses have been added to the pool since the initial purchase.

From the outset, we were fortunate enough to obtain a floating network license (FNL) as our initial license purchase. This has turned out to be very beneficial to us, and we highly recommend this option if you can possibly afford it. The advantages of the FNL include: (1) installation of the software on any number of computers and platforms as long as it is available to the license server within the local-area network (LAN), (2) connecting the local desktop as a client, and a remote, perhaps more powerful, computer as the server only uses a single license and offloads the computation so that the desktop is available for other tasks, and (3) if you have a cluster computer available, you can connect any number of compute nodes with a single network license.

The criteria required to obtain a “site” license of COMSOL at ORNL are not easily achieved. In the last few years, we have become organized and, with COMSOL cooperation and permissions, have been able to pool resources with other ORNL divisions in order to save money, and combine licenses together into a larger pool of licenses. Through the use of a license plan, the pool members agree on the license distribution, and we have been

able to allocate the licenses fairly across many machines and users. Our peak time is usually midday during the midsummer months when we have many visiting summer interns from Universities all over the USA. Both mentor and students find COMSOL to be a valuable resource to get something accomplished in a short time while here during the summer months. Often, it is necessary to ask people to reduce license usage in order to get the normal work done during these peak times. As long as we follow the plan, we have not had many problems in license allocation. We have also not had many problems with unapproved users from the LAN. We want to encourage new users, and gain colleagues through the common interest of COMSOL, but we also want to make sure there is no abuse of our licenses taking place. It is fairly easy to spot such rare occurrences using the license manager tools provided with the software.

Early versions of COMSOL came with a hardcopy set of manuals to provide code documentation. The COMSOL documentation is entirely electronic now, and can be optionally downloaded with the software. The installation media was originally provided as CDs, then DVDs for a short while, but now is entirely downloaded from the company. We have found the .iso files very convenient for quick and clean installations across many platforms and machines on our LAN. We use the same license manager server to store local copies of all the code installation media, license files, documentation, training materials, and anything associated with the code in one place. I have developed local update scripts that allow me to download a single instance of the COMSOL application library, and updates, and then patch the other machines very quickly across the LAN. This allows all the machines and documentation to be kept up to date in a timely manner, and without major effort. We could improve on this by using network file systems (NFS), and we hope to do this in the future.

6.2 Local COMSOL User Group

We started the concept of a local COMSOL user group here at ORNL. The most difficult issue to overcome is finding out who else at ORNL also had licenses. ORNL is a large organization with over 5000 employees, contractors, guests, interns, etc., many of whom are involved in computer simulation of varying levels of complexity. We obtained a list of local users and interested people, sent out e-mail notifications, and also announced in our local ORNL "technical calendar." We would meet in various locations around ORNL. Our discussions usually would center around one person's experiences or results, and move into questions and answers about the software.

This approach worked for a while, but we now have enough local users that work regularly with COMSOL, such that, a "critical mass" of individuals are always available. In this manner, the user-group meeting can always morph into a project meeting about the current COMSOL

work that is going on. This type of arrangement is particularly useful if we have a number of students who are working with the staff for their graduate research, and can use this meeting time to convey their work to their mentors and peers. Our COMSOL user group meeting continues to meet about once per month, and now regularly includes COMSOL users from outside ORNL, including other DOE facilities in Oak Ridge.

This type of personal interaction with other ORNL users helps to get our COMSOL work for ORNL done in a more efficient manner, develop new colleagues in related areas, learn what others are doing at ORNL, helps to increase the membership of our license pool, and of course, learn new things about how to use COMSOL.

6.3 Joint ORNL / COMSOL Symposia / Workshops

We have conducted a joint ORNL and COMSOL symposia and workshop several times at ORNL. The event is conducted by having a set of several presentations in the morning hours with results and experiences from local ORNL users, followed by a routine workshop led by a COMSOL representative in the afternoon. This all-day free event brings in interested people from within and outside ORNL to witness first hand what COMSOL is all about, and learn and ask questions about the applications and the code. We have found this particularly useful for graduate students to showcase their work, and give them valuable experience in presenting their work to technical groups who may quiz them about their work. All attendees will learn something new about COMSOL, particularly if the event coincides with the release of a new version of the software. We have held the event at different locations, but have settled on having it in one of the large meeting rooms in the main ORNL visitor center, which is conveniently located just above the main ORNL cafeteria; a great location for lunch and / or breakfast to accompany the event. It is some work to setup the event, and the normal process for people outside ORNL to visit ORNL must be followed, but nevertheless, we have had much success with this type of event. We usually hold this on an annual basis, but it has been a while since the last event due to conflicts with our schedules.

6.4 Local Tips and Tricks

As we have evolved as a group of COMSOL users, and even with my own personal experiences in using COMSOL, we have found that often times, we repeat the same need for help, or repeat the same mistake. In our COMSOL user group meeting, a participant would mention "we need to write that down so we won't forget it." This has especially occurred when new users arrive to our license pool; even if experienced with COMSOL in the past. There is plenty of help available from the COMSOL web site, or through their technical support team, but this type of help

is specific to our local installation. Hence, the need arose, and we started a list of “local tips and tricks” for using the COMSOL software with our license pool. The list consists of a collection of portable document format (.pdf) files in a directory (or folder) stored on the same machine that is our COMSOL license server, as well as data archive. Since the directory is also available through a web server, we can simply send the user who needs help a web link to the tip description. Our collection is currently very short, but examples of our local tips and tricks are:

- A recovery file example to plot while running from a remote machine,
- How to use the CAD import license wisely,
- How to link to the local application, parts, and documentation library to avoid downloading,
- How to use the new numasets switch setting for a performance boost,
- How to use the LaTeX and TeX family of math and symbol fonts in your COMSOL plots, and
- Tips for cluster computing and setting memory limits for COMSOL to avoid cluster crashes.

We have several tips and tricks we could add to our list, but need the time to make it happen.

6.5 Software Quality Assurance

We are required by our primary customer, the US Department of Energy (DOE), to comply with certain software quality assurance (SQA) requirements for all software we use. Not all software falls in the same level of oversight, and because our primary purpose for using COMSOL is to support the operation of the HFIR, which is a nuclear facility, we fall under a very high-level of oversight. We separate our SQA efforts into two categories: (1) verification, and (2) validation, or V&V. We have developed procedures over the years to deal with these requirements, our DOE customer has audited these procedures, and we follow those procedures when we use COMSOL to provide detailed analysis for design, safety, or operations analysis of a system, structure, or component within the HFIR.

Compliance with the validation requirements can be the most difficult to meet since the ideal situation is to have experimental, test, or operational data to directly compare and measure the code accuracy. Often, the right data is not available, and we must reduce our expectations, and instead, compare our results to that of another computer code, or the same code with a completely independent model. This can also be difficult, because the comparison code may not have all the capabilities that the reviewed code has. Lastly, if no data or comparison code is available, an expert opinion is obtained, in which case, the usual steps are to perform a conservative analysis to arrive at a worst case, and see if the reviewed code results are within that level of conservatism or other rational approach to accept the results. The best approach, and one which we are working on presently for COMSOL, is to

produce a stand-alone validation document that demonstrates valid results for a number of situations, such that, the findings can be applied to a number of situations.

Compliance with our verification requirements are more straight forward. In a nutshell, we are required to “demonstrate that the code is installed correctly, and produces the results that were intended by the code developer.” So, in the case of COMSOL, we are provided a number of model files from the application library. We pick several of these models out that are similar in application to what we intend to use COMSOL for in HFIR, and we reproduce the results that are documented and provided in electronic form as solutions by the COMSOL developers. It is important to note that, if we pick the verification models wisely, they can also serve as validation results since many of the COMSOL application library models contain high-quality, and reference-able data by which to compare. In addition, we are also required to keep a tight configuration control on both our hardware and software so that changes in the operating system (OS) or hardware do not cause changes in the verified results after the initial installation. Prior to version 5.0 of COMSOL, we demonstrated compliance with our verification procedures, by manually going through the process, i.e., “by hand,” for versions 3.5a, 4.2a, and 4.3.[2] Starting with version 5.0, a new automated procedure has been developed and exercised and satisfied all requirements, and is the subject of another paper and poster in this conference[19]. We anticipate that COMSOL will release new tools that allow for a similar, and perhaps superior, verification compliance capability for all COMSOL users in the future.

7 Suggestions and Conclusions

COMSOL is a complex tool and having used it for a number of years now, we do not think any one person knows everything about the entire code package. As such, keeping up with the capabilities and learning more about COMSOL becomes a continuous process. With each meeting, workshop, or conference, there is always something new you can learn about COMSOL that will make your modeling and simulations efforts of higher quality, more efficient, and more useful to others. We also think that it is beneficial to have several colleagues using COMSOL together to learn from each other, and become better at what you do through joint efforts, peer review, and constructive debate and criticism. Often, there is no one best way to accomplish your goals when using COMSOL, so help from your local peers, followed by help from COMSOL technical support is essential to help you reach your modeling and simulations goals.

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perienced professional colleagues who are starting to become COMSOL users; Drs. Michael W. Crowell and Emilian L. Popov in the areas of software quality assurance and input data validation and documentation respectively. And finally, I would like to acknowledge colleagues Franklin G. Curtis (PhD student and ORNL staff member), and Christopher J. Hurt (PhD student, and part-time staff member) for their many contributions in this working group. Both Franklin and CJ are using COMSOL to support their graduate degrees. Prashant, Mike, and CJ have separate papers and posters in the conference this year (2015 Boston).

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