The e-cam Issue

What are "simulations" in advanced research? Is HPC the Holy Grail of scientific simulations? Let's find out together!

Comics & Science

WHERE ENTERTAINMENT AND SCIENCE MEET

e-cam

CENTRE EUROPÉEN DE CALCUL ATOMIQUE ET MOLÉCULAIRE
cecam
SINCE 1969

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Comics & Science

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INTRO

There is a reality permeating our world but still invisible to the general public.
Today, our understanding of the physical world relies on sophisticated mathematical tools and this is taken for granted. What is much less obvious is "how" this takes place. It's a recipe including at least two crucial ingredients: 1) mathematical models portraying reality in a simplified, accessible way; 2) computational methods allowing us to compute solutions to those models. In order to clarify what actually happens when these two ingredients mingle together, a considerable degree of abstraction is needed. The standard solution to this dilemma in scientific communication is to simply jump past the obstacle, telling stories about the final result: a new drug molecule; an "esoteric" material with never-before-seen properties; the "intelligent" fluid. This book has been produced in partnership with CECAM–Centre Européen de Calcul Atomique et Moléculaire and the EU funded E-CAM project as an attempt to make that "how" clearer. With this in mind, cartoonists Giovanni Eccher and Sergio Ponchione tell a story where the "philosophy of models" and the powerful ingredient that is HPC–High Performace Computing, are explained in a – hopefully – easy-to-understand way.

Roberto Natalini
Andrea Plazzi

The e-cam Issue

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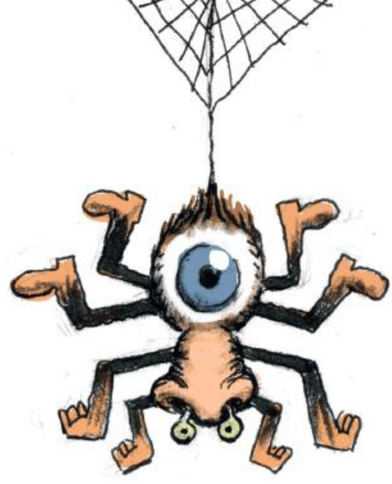


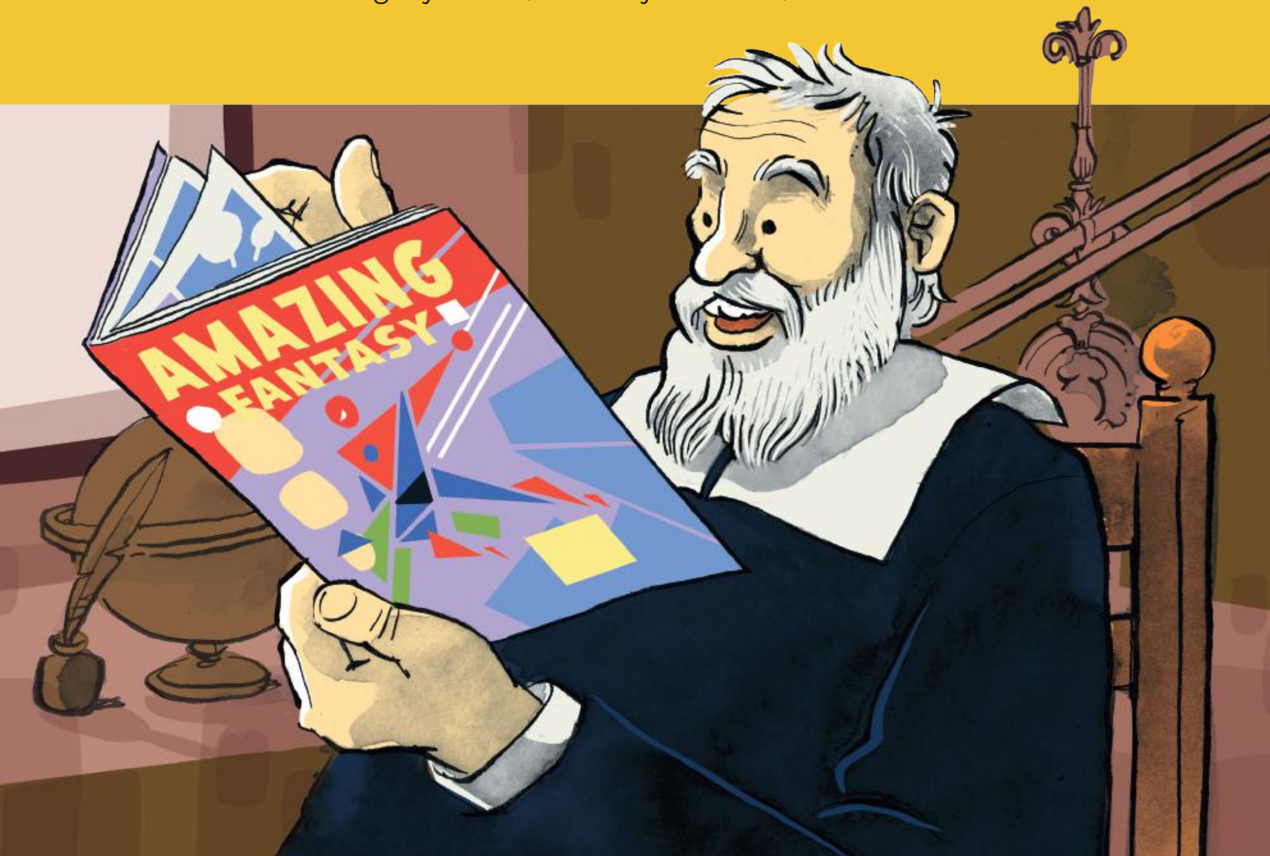
DEAR CURIOUS READER...

IGNACIO PAGONABARRAGA
SARA BONELLA

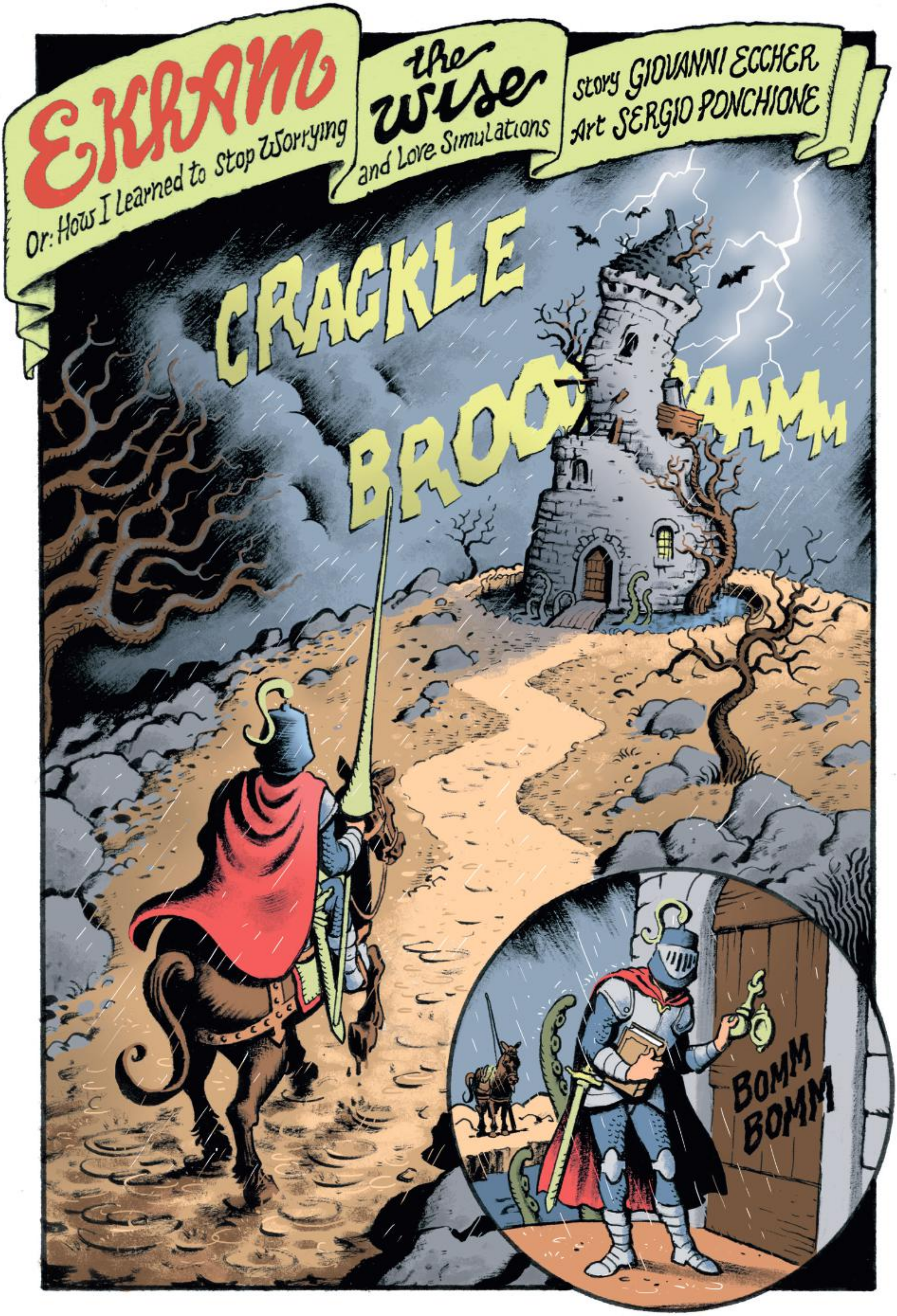
"*The book that is continuously open in front of us (I mean the universe)... is written in a mathematical language, and its characters are triangles, circles and other geometrical figures*" (Galileo Galilei). This idea has shaped science for about four centuries: generations of scientists, giants and dwarves standing on their shoulders, have advanced by expressing the laws of nature as mathematical equations. Modern physics, chemistry, engineering, even biology, are dialects of this elegant language. There is just one tiny problem: almost all the equations used in science can be *written* but not *solved*! Much can be learned from qualitative or approximate treatment of the equations, but the situation is embarrassing, a bit like having a book and not being able to decipher it beyond its index. Wouldn't it be better to unlock its chapters and read pages and words? Surely, our understanding of the story, our ability to predict its twists and turns, and the fun we have with it would grow with each layer! With some luck, we might even discover that the book contains blank pages yet to be filled with new characters of our own creation. If we stop at the equations we are blind to these exciting possibilities. In the middle of the 20th century, scientific use of computers gave us new glasses, powerful enough to read past the index. From the first machines to today's high performance computers, our new glasses have become more and more precise. Harnessing their growing power via increasingly sophisticated algorithms, we can now calculate approximate solutions for the equations that are virtually indistinguishable from the – inaccessible – exact ones. Even better, we can control the quality of our approximation, assess when to trust it, try to improve it systematically. Better still, respecting general mathematical laws, we can use computational tools to model nature and simulate its behavior under controlled circumstances with unprecedented flexibility, not bound by the restrictions imposed by experimental setups in a laboratory. And we can do this, crucially, knowing that we are creating an image of the world that – like any theory – has limitations and boundaries. Using computers to make theory, then, we can access chapters, pages, words, and move, hopefully, one step closer to understanding the book of nature. This is the tale that we try to tell in this issue.

Naturally, our story does not exhaust the field of simulation and modelling, and simulation and modelling does not exhaust the scientific method. Furthermore, a scientific answer usually begets a new scientific question, so no scientific tale has a real ending. But there is power within this incomplete understanding: if the image of our simulation is accurate enough, we can use it to affect – not only understand – the world. We can build an opportunity to turn our understanding into a tool to create a safer, more sustainable future and to improve our lives. The ultimate outcome of this process, of course, depends on factors and choices that cannot be expressed, interpreted, let alone governed, with mathematics or computers. "*With great power comes great responsibility*" (Peter Parker, to a first approximation), but this – key - point, dear Curious Reader, is the beginning of another story...

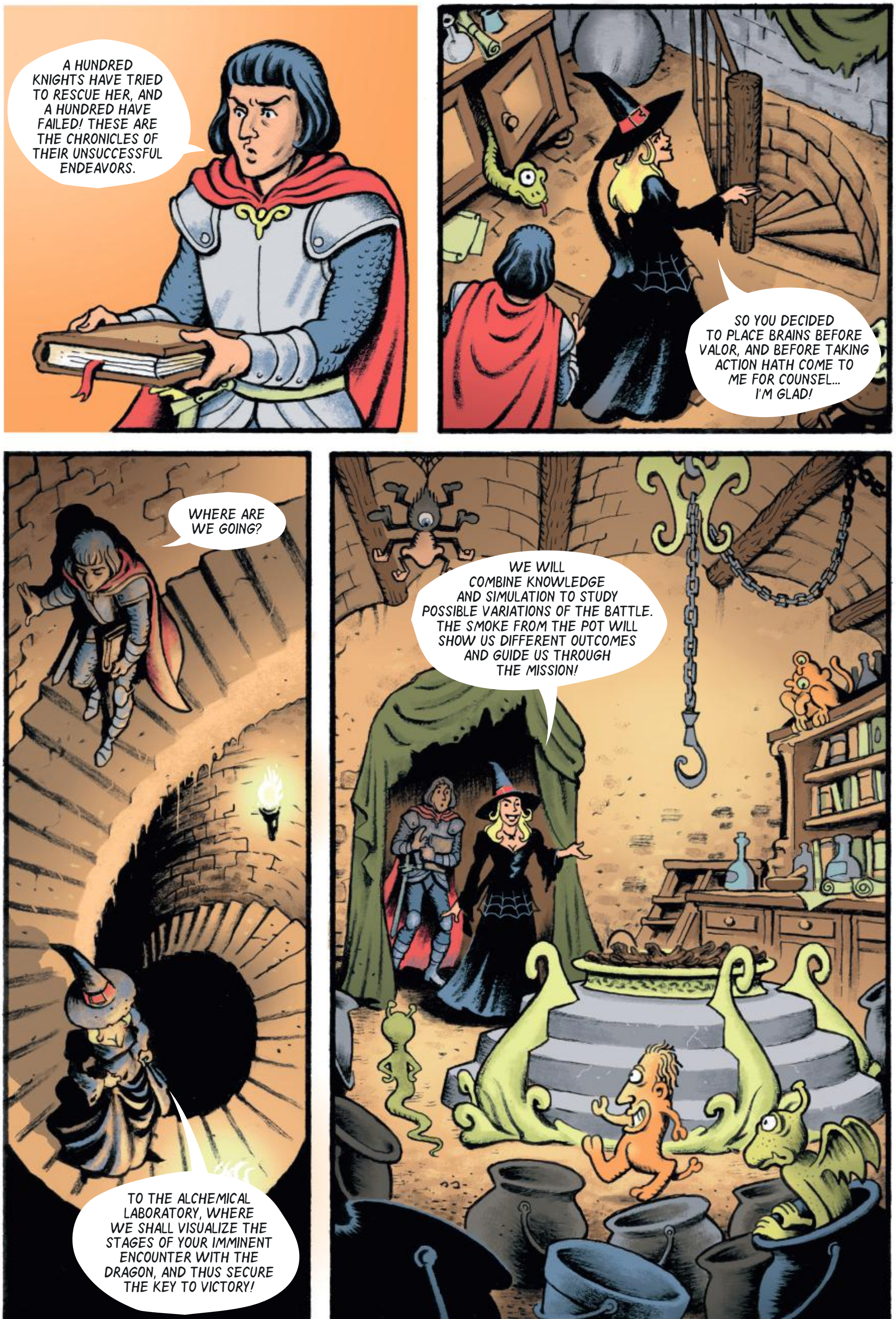
For the time being, we hope that you will enjoy this introduction to the world of simulations as much as we enjoyed creating it with Comics&Science. To their wonderful team goes our warmest thank you for the talent, craft, and patience that carried us through this slightly bizarre, but really wonderful, adventure!

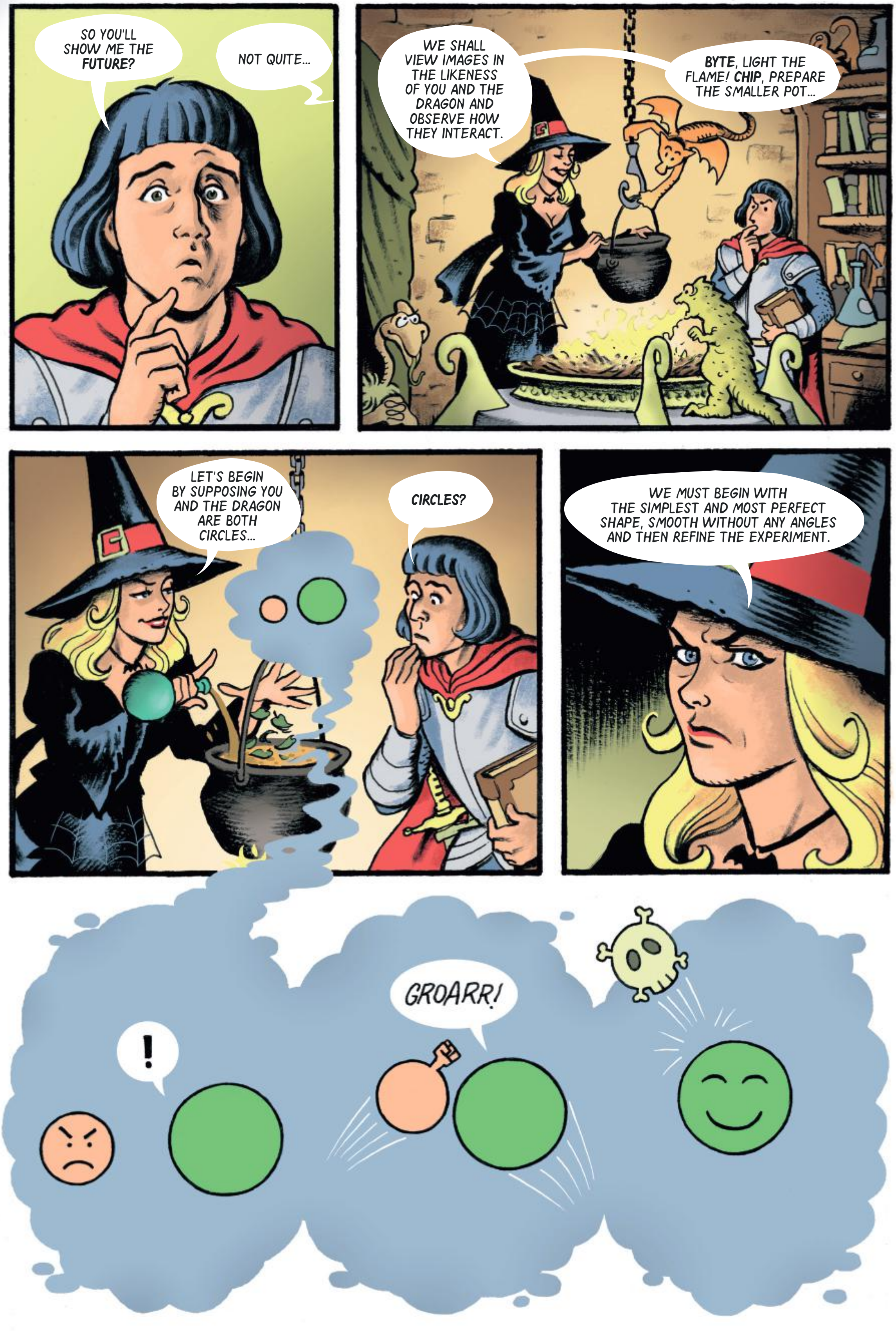


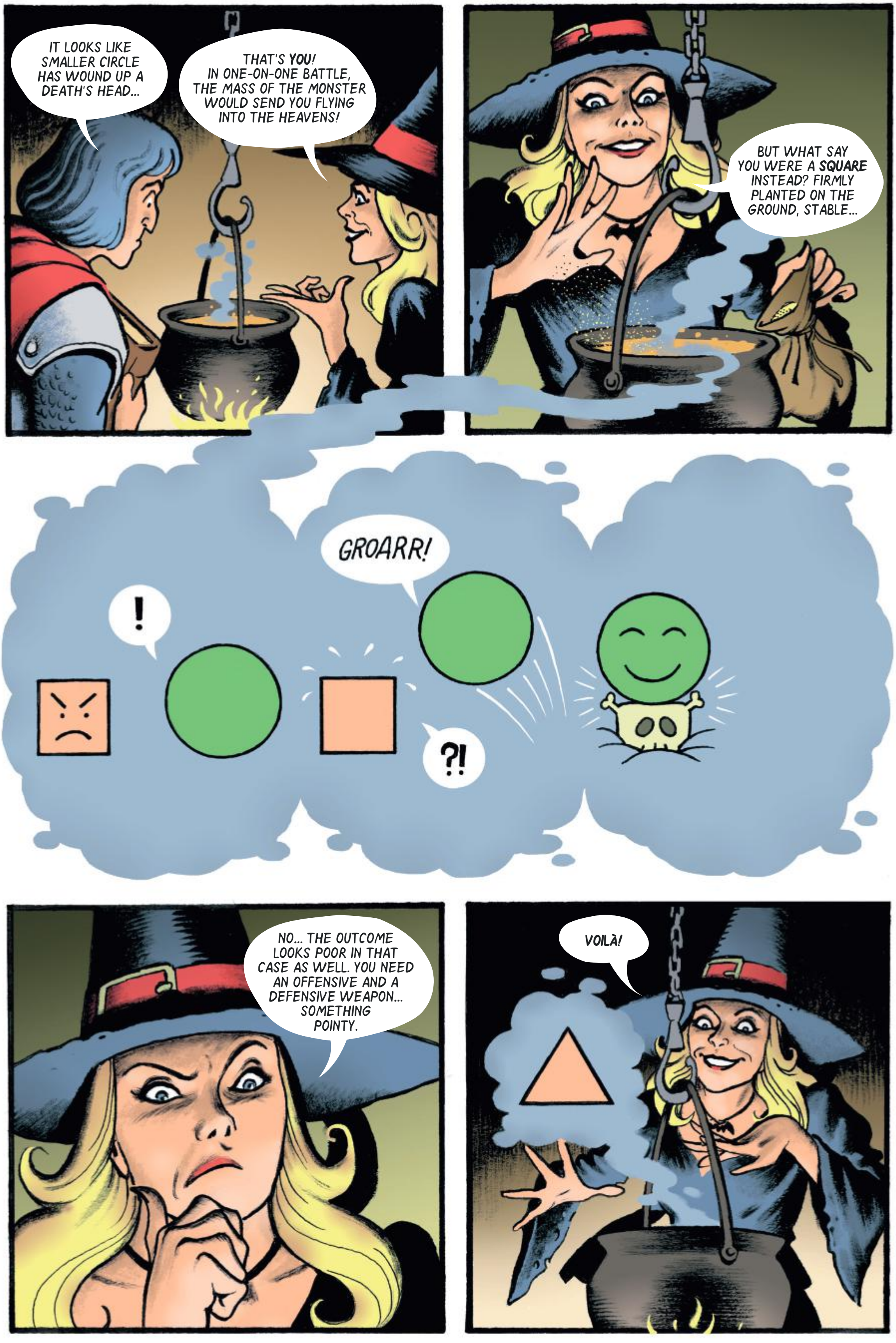

HPG

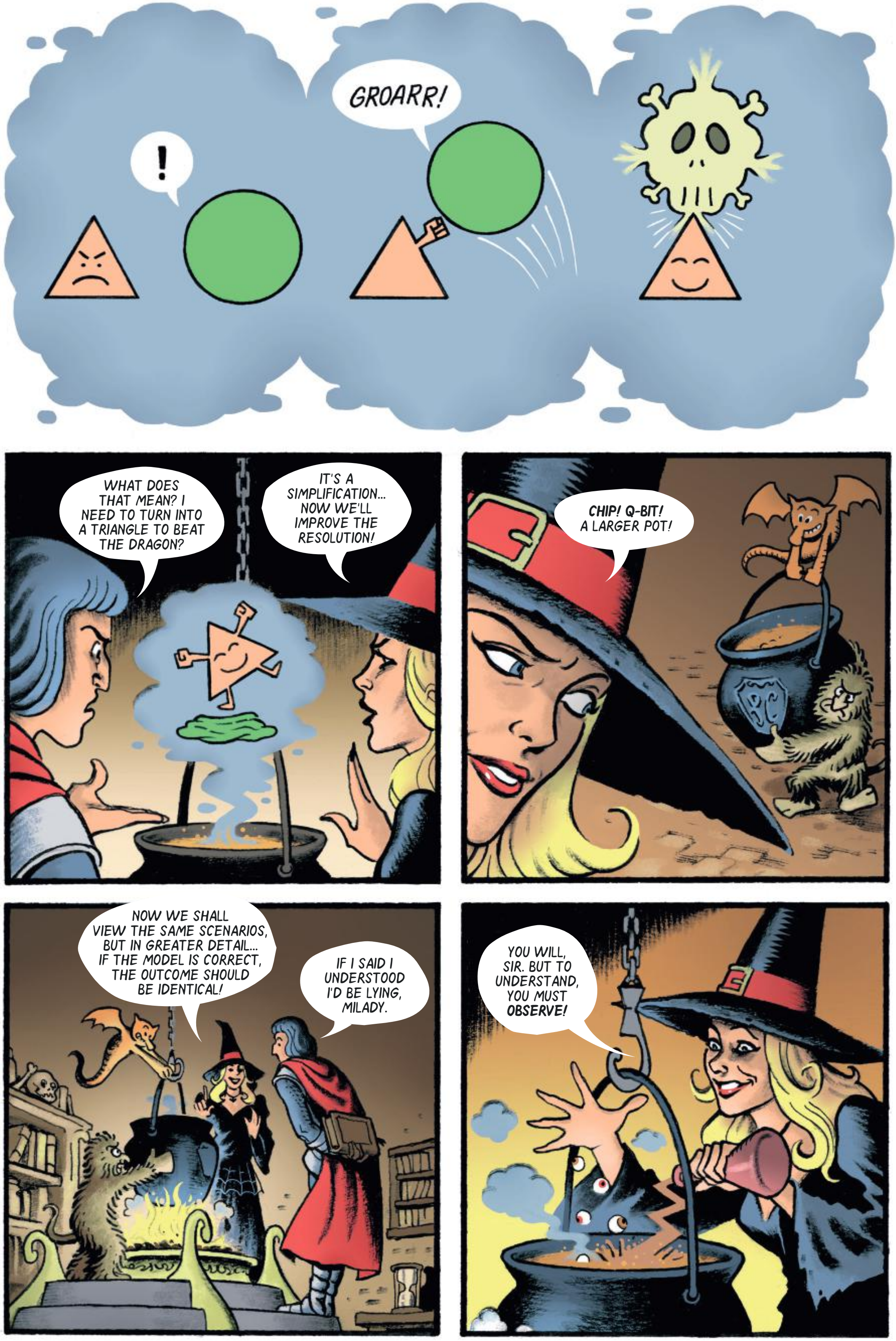

EKRAM the wise
Or: How I Learned to Stop Worrying and Love Simulations
story GIOVANNI ECCHER
Art SERGIO PONCHIONE
CRACKLE
BROO
AAMMM
BOMM
BOMM

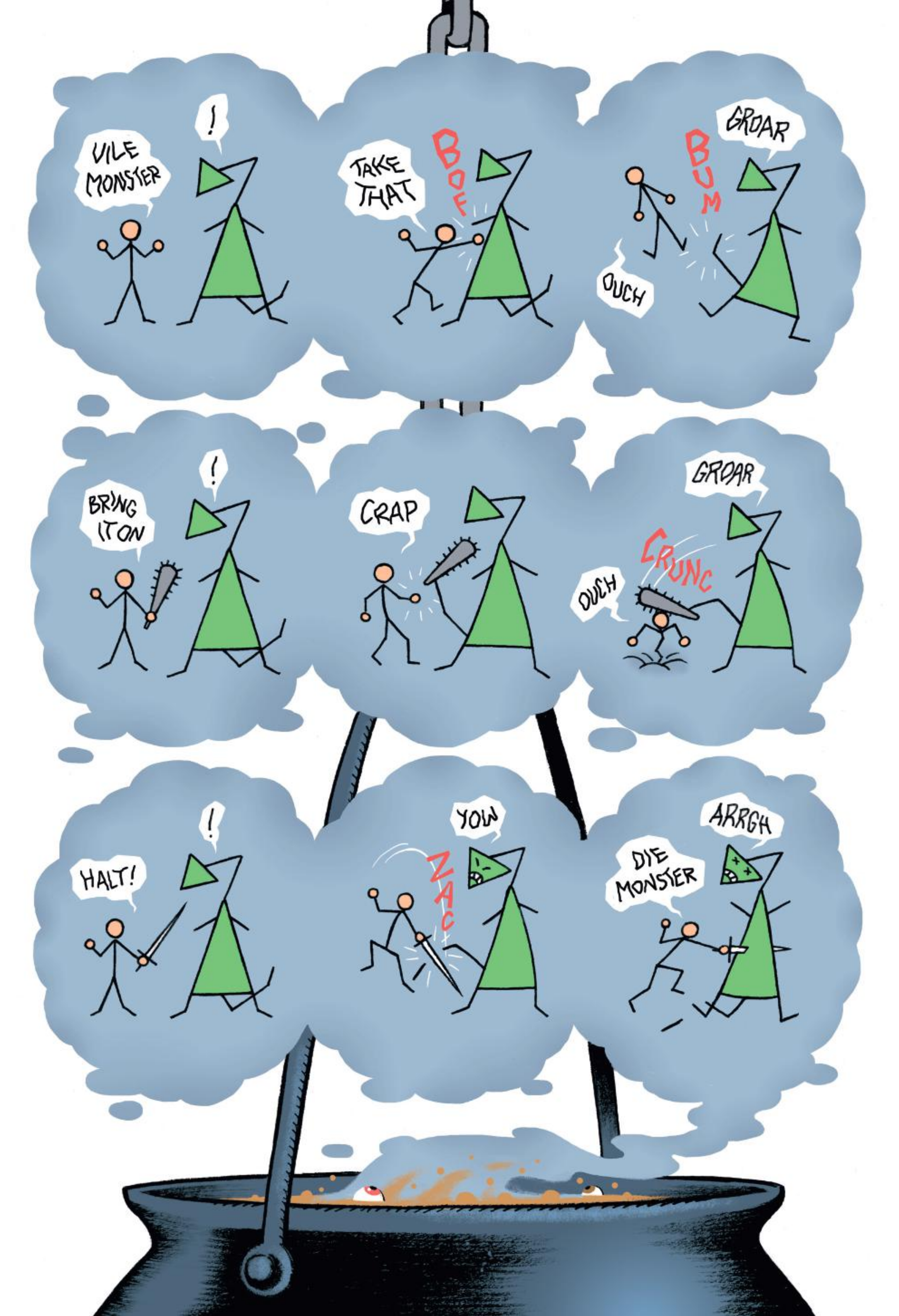
PRINCE VARIANT! I'VE BEEN EXPECTING YOU... COME IN, LEST THE OXIDE RUINS YOUR ARMOR!
YOU KNEW I WAS COMING, ECLECTIC EKHAM? HOW...?
HEY, IF I COULDN'T TELL THE FUTURE, YOU WOULDN'T HAVE COME LOOKING FOR ME.
YOU'RE RIGHT, MILADY. I'VE COME TO ASK FOR YOUR HELP. PRINCESS BEAUTY HAS BEEN KIDNAPPED BY A TERRIBLE DRAGON, AND...
AND HER FATHER, THE KING, HATH PROMISED HER HAND AND HALF THE KINGDOM TO THE PERSON WHO RESCUES HER.
INCREDIBLE! EVERYTHING THEY SAY ABOUT YOU IS TRUE!
IT'S NOT LIKE IT TAKES A PROPHET. THAT'S THE STANDARD PROCEDURE FOR A PRINCESS IN TROUBLE.


A HUNDRED KNIGHTS HAVE TRIED TO RESCUE HER, AND A HUNDRED HAVE FAILED! THESE ARE THE CHRONICLES OF THEIR UNSUCCESSFUL ENDEAVORS.
SO YOU DECIDED TO PLACE BRAINS BEFORE VALOR, AND BEFORE TAKING ACTION HATH COME TO ME FOR COUNSEL... I'M GLAD!
WHERE ARE WE GOING?
TO THE ALCHEMICAL LABORATORY, WHERE WE SHALL VISUALIZE THE STAGES OF YOUR IMMINENT ENCOUNTER WITH THE DRAGON, AND THUS SECURE THE KEY TO VICTORY!
WE WILL COMBINE KNOWLEDGE AND SIMULATION TO STUDY POSSIBLE VARIATIONS OF THE BATTLE. THE SMOKE FROM THE POT WILL SHOW US DIFFERENT OUTCOMES AND GUIDE US THROUGH THE MISSION!


SO YOU'LL SHOW ME THE **FUTURE?**
NOT QUITE...
WE SHALL VIEW IMAGES IN THE LIKENESS OF YOU AND THE DRAGON AND OBSERVE HOW THEY INTERACT.
BYTE, LIGHT THE FLAME! **CHIP**, PREPARE THE SMALLER POT...
LET'S BEGIN BY SUPPOSING YOU AND THE DRAGON ARE BOTH CIRCLES...
CIRCLES?
WE MUST BEGIN WITH THE SIMPLEST AND MOST PERFECT SHAPE, SMOOTH WITHOUT ANY ANGLES AND THEN REFINE THE EXPERIMENT.
!
GROARR!


IT LOOKS LIKE SMALLER CIRCLE HAS WOUND UP A DEATH'S HEAD...
THAT'S **YOU**! IN ONE-ON-ONE BATTLE, THE MASS OF THE MONSTER WOULD SEND YOU FLYING INTO THE HEAVENS!
BUT WHAT SAY YOU WERE A **SQUARE** INSTEAD? FIRMLY PLANTED ON THE GROUND, STABLE...
!
GROARR!
?!
NO... THE OUTCOME LOOKS POOR IN THAT CASE AS WELL. YOU NEED AN OFFENSIVE AND A DEFENSIVE WEAPON... SOMETHING POINTY.
VOILÀ!


!
GROARR!
WHAT DOES THAT MEAN? I NEED TO TURN INTO A TRIANGLE TO BEAT THE DRAGON?
IT'S A SIMPLIFICATION... NOW WE'LL IMPROVE THE RESOLUTION!
CHIP! Q-BIT! A LARGER POT!
NOW WE SHALL VIEW THE SAME SCENARIOS, BUT IN GREATER DETAIL... IF THE MODEL IS CORRECT, THE OUTCOME SHOULD BE IDENTICAL!
IF I SAID I UNDERSTOOD I'D BE LYING, MILADY.
YOU WILL, SIR. BUT TO UNDERSTAND, YOU MUST OBSERVE!


VILE MONSTER
!
TAKE THAT
BOF
GROAR
BUM
OUCH
BRING IT ON
!
CRAP
GROAR
CRUNC
OUCH
HALT!
!
YOW
ZAC
ARRGH
DIE MONSTER


NOW IS THE PROJECTION CLEARER, GOOD SIR?
I THINK SO...
IT SEEMS THAT THE BEST WEAPON TO VANQUISH THE DRAGON IS A SWORD... BUT MANY OF THE KNIGHTS WHO WERE DEFEATED CARRIED ONE!
SEVERAL VARIABLES ARE STILL MISSING... BUT THIS **HIGH PERFORMANCE CAULDRON** IS SO POWERFUL, WE CAN ADD THEM TO THE COMPUTATION TO IMPROVE THE SIMULATION FURTHER!
DID YOU NOT SAY THAT BOOK CONTAINS THE ENDEAVORS OF THE DEFEATED KNIGHTS?
YES, OR AT LEAST WHAT'S KNOWN OF THEM...
LET'S SEE... BADUMPH THE LARGE, IMPALED BY THE BEAST'S TAIL...
GUNDRAK THE IMPERVIOUS, BURNED BY THE DRAGON'S FIERY BREATH... A CLASSIC!

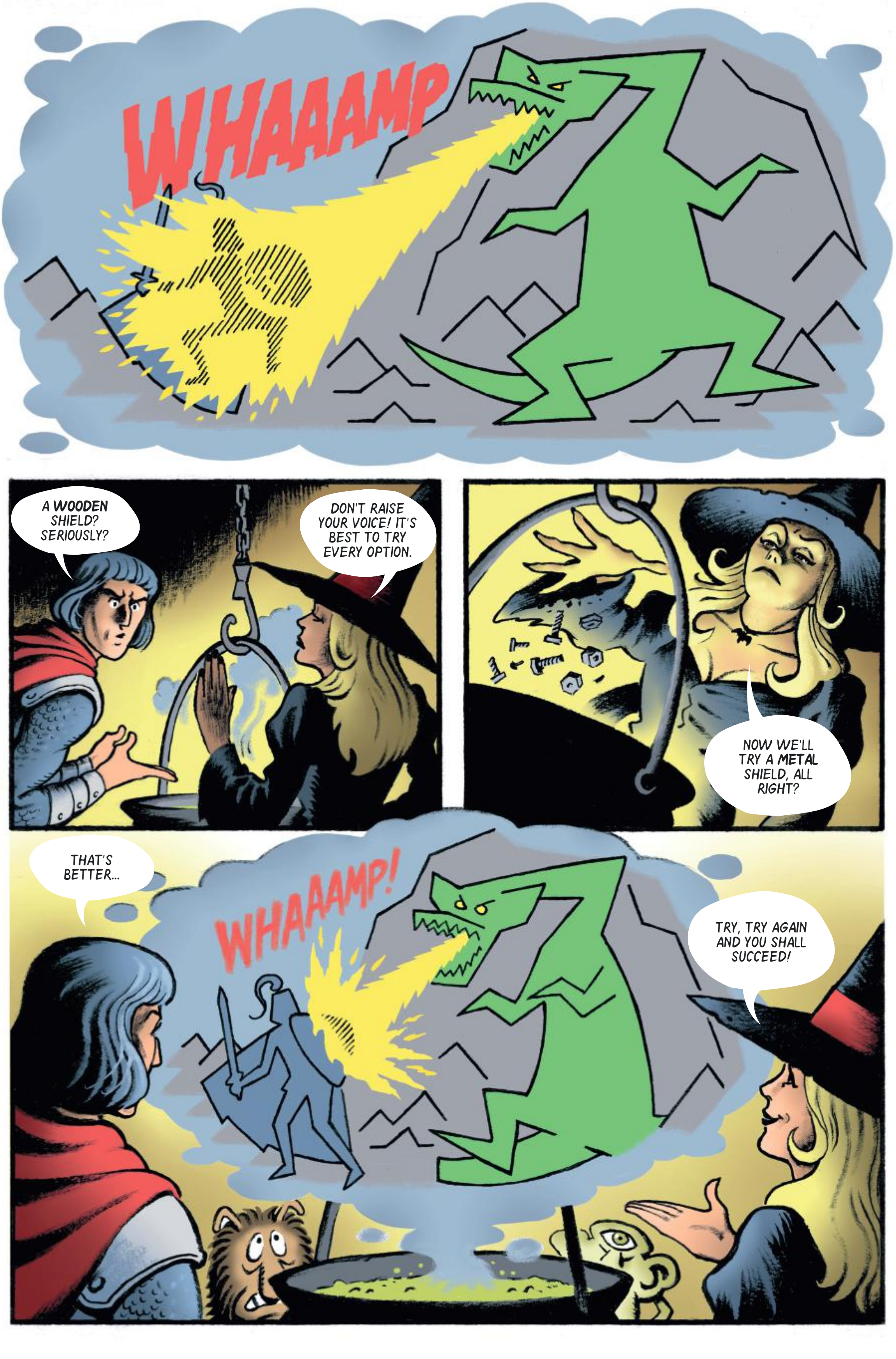

LET'S ADD THIS INFORMATION TO THE POT AND YOU'LL SEE THE FIGURES TAKE SHAPE... JUST LIKE YOUR FATE!
THERE! BUT WHAT'S...
BOOM


WHAT... WHAT HAPPENED?
SOMETHING WENT WRONG... AND I'M AFRAID I KNOW **WHAT!**
WHEN YOU'RE WORKING WITH SUCH SOPHISTICATED CAULDRONS, IT TAKES LITTLE TO BOTCH A SIMULATION...
LIKE THIS **BUG!** SOMEONE DIDN'T CLEAN THE LAB VERY WELL, DID THEY, **CHIP?**
BAH! CLEAN UP THIS DISASTER, SERVANTS OF ILL OMEN, AND WE'LL RESUME THE SIMULATION!


UH... MAYBE I'LL STAND BACK A LITTLE THIS TIME! ARE YOU SURE IT WON'T EXPLODE AGAIN?
NOTHING IS SURE IN THIS WORLD, PRINCE. THAT'S WHY THERE ARE SEERS LIKE ME! NOW COME CLOSER...
BRING IT ON, DRAGON!
ROARRRGHH!
AAAGH!


TOO SLOW, BUDDY...
TUMP
RRARRGH!
WHACK
AND NOW, PREPARE TO DIE...
WHAMMP

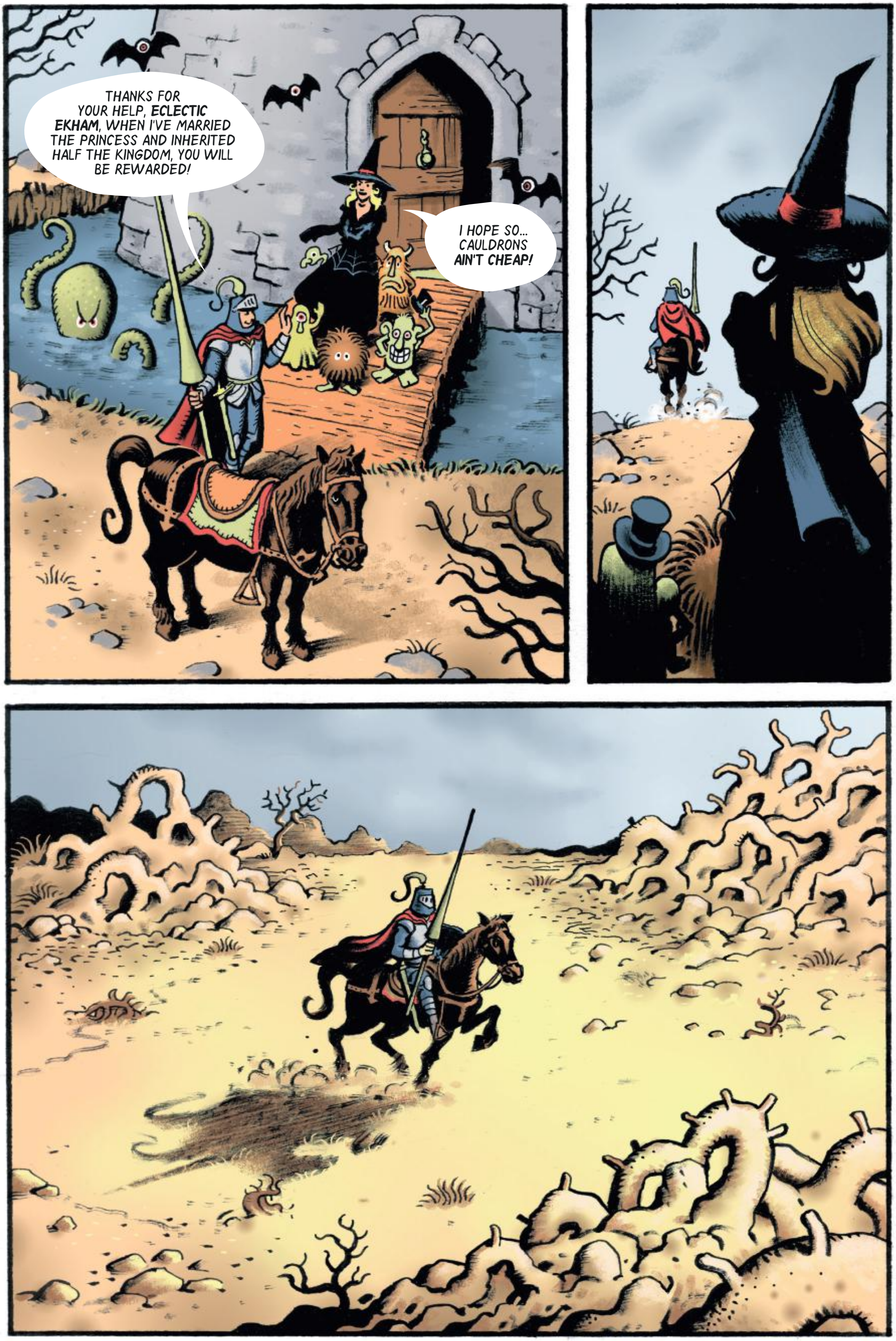

W-WHAT? WASN'T I SUPPOSED TO **WIN?**
INTRODUCING NEW VARIABLES CAN CHANGE THE RESULTS... THAT'S WHY WE'RE DOING A SIMULATION.
FOR EXAMPLE, LET'S TRY ADDING A **SHIELD...**
HA HA! DO YOUR WORST, BUDDY...


WHAAAMP
A WOODEN SHIELD? SERIOUSLY?
DON'T RAISE YOUR VOICE! IT'S BEST TO TRY EVERY OPTION.
NOW WE'LL TRY A METAL SHIELD, ALL RIGHT?
THAT'S BETTER...
WHAAAMP!
TRY, TRY AGAIN AND YOU SHALL SUCCEED!


YAAH!
WHAM
WHACK
RRAAAGH!
GREAT! SO THAT'S HOW I'LL DEFEAT THE MONSTER?
BE PATIENT, WARRIOR... WE MUST REPEAT THE EXPERIMENT UNTIL WE REACH THE HIGHEST LEVEL OF DETAIL MY CAULDRONS PERMIT!


ONLY **THAT** WAY WILL WE BE SURE... BUT REMEMBER, WHAT YOU SEE HERE IS **NOT** REALITY, ONLY ITS LIKENESS!
SO I COULD FAIL, NO MATTER WHAT?
NO! IF VISION AND REALITY ARE CLOSE ENOUGH, THEY WILL BECOME ONE AND THE SAME...
THAT'S WHY WE MUST ADD ALL THE VARIABLES WE KNOW OF, OBSERVE AND TRY AGAIN!
AGAIN... **AND AGAIN!**
WHAMP


SWISSS


THANKS FOR YOUR HELP, ECLECTIC EKHAM, WHEN I'VE MARRIED THE PRINCESS AND INHERITED HALF THE KINGDOM, YOU WILL BE REWARDED!
I HOPE SO... CAULDRONS AIN'T CHEAP!


RECKONING TIME, **DRAGON!** COME OUT OF THAT CAVE AND FIGHT LIKE A ***MAN!***
RROAAARRRGH!


VICTORY! THANK YOU, WISE EKHAM...
PRINCESS, YOU'RE FREE! I SHALL RETURN YOU TO YOUR FATHER'S CASTLE, WHERE WE WILL MARRY AND LIVE HAPPILY EVER AFTER!
SHALL WE NOW?
WHAT ARE YOU SUGGESTING, MILADY? I SAVED YOU FROM THE FIERCE DRAGON, YOUR FATHER PROMISED THAT...
MY FATHER DOES NOTHING BUT GIVE MY HAND IN MARRIAGE LEFT AND RIGHT! WHY DO YOU THINK I'M HIDING OUT HERE?
TO GET AWAY FROM MEN LIKE YOU! IF I EVER DECIDE TO GET MARRIED, I'LL DECIDE TO WHOM!
BUT THE DRAGON...


I TRAINED THE DRAGON MYSELF, TO DETER THESE CHUMPS... **DO YOU HAVE ANY IDEA HOW LONG THAT TOOK?**
I GUESS THIS WAS BOUND TO HAPPEN SOONER OR LATER... WELL, DO YOU HAVE A HORSE TO RIDE BACK ON, AT LEAST?
OF COURSE! TRUSTY BUCEPHALUS! YOU CAN HOLD ON TO ME AS I RETURN YOU TO YOUR ANCESTRAL HOME, AND MEANWHILE...
MEANWHILE I BID YOU **ADIEU**, BUDDY! YOUR HORSE FOR MY DRAGON, NOW WE'RE EVEN...
HEY!
MY LOVE! DON'T GO... **HUFF!** WE BELONG TO EACH OTHER! IT'S THE LAW OF CHIVALRY! **HUFF!**


OH, WISE EKHAM! THE PRINCESS RAN OFF, TAKING MY HEART AND HORSE WITH HER. YOU MUST HELP ME TO FIND HER!
I'M SORRY, SIR, BUT I'M VERY BUSY... COME BACK IN A YEAR OR TWO, EH?
IS HE GONE?
I HOPE SO... YOU'RE RIGHT. HE IS PERSISTENT!
BUT I'LL HELP YOU ESCAPE THIS ODIOUS UNION...
HOW, OH MIGHTY EKHAM?
TRYING AND TRYING AGAIN, WITH THE HELP OF MY MAGIC POTS! WE'LL BEGIN BY PICTURING YOU AND THE PRINCE AS A PAIR OF CIRCLES...
CIRCLES?
...

A **conversation** about how "it all came to be".
Or: how **researchers** and **cartoonists**
found a way to **tell laypeople** about
what many scientists actually do and why.

Simulating simulations. With comics

CECAM
COMICS&SCIENCE

Andrea Plazzi To start with, where does this far-fetched idea of a Witch, a Brave Knight, a Princess in distress and a Dragon come from?

Giovanni Eccher From a trip in the mountains. It was just one of the ideas I was playing with... there were three or four other options. In the end, we settled for this one.

AP Computer simulation and High Performance Computing (HPC) are very specialized and abstract fields. What did CECAM want to tell the general public about them, and why?

Ignacio Pagonabarraga This was kind of an adventure for us. In the first place, we don't have the experience to tell a wider audience what we do. And what we do, it's not "physical"... it's something more conceptual. We use machines, but they are only tools. So we needed to convey this message: what modelling and simulation are, why they are so important, and the need for HPC infrastructures. The framework is the E-CAM project, which is about the development of scientific software in HPC environments. I remember how in the beginning we had very open, and to some extent, heated discussions, trying to find a common language. It was a great challenge for us.

AP Why did you find the *Comics&Science* format appealing?

Sara Bonella I discovered *C&S* while visiting CNR-IAC Director Roberto Natalini in Rome. Actually, I remember our first conversation very well... his enthusiasm surprised and enthralled me, not to mention the posters hanging in his office. At the same time, Ignacio

was stressing how we needed a way to broadly communicate our work in E-CAM and in CECAM (the institute coordinating E-CAM as a European project). At first we had no idea about how to go for it, and we really have to thank Roberto, and Giovanni of course, for their patience in putting up with us when we were trying to explain simulation and modelling. And then Sergio for shaping our ideas so nicely. We were looking for innovative and funny ways to disseminate what's behind our projects and when we saw *C&S*, we jumped on it.

Roberto Natalini Actually, you were asking for something we had been looking for before you, when Andrea and I started wondering what kind of medium (although comics was quite a natural choice, because Andrea is a huge expert) would be the best to communicate science. This is a very big problem for all institutions. At CNR-Consiglio Nazionale delle Ricerche – the public research institution I work for – and IAC, my institute, a mathematical institute, we have this problem: how to tell the general public, what we do, what our work, our daily routine is when we go to the institute. My own children, they once said my job was to spend time on the phone! It is really difficult to explain what mathematicians, theoretical physicists, or computational physicists do in their daily jobs. Really, really difficult. And comics have this quality: they are inherently flexible and easy. That's why I turned my office into a *Comics&Science* club, with posters everywhere as a marketing strategy, you might say.

AP Sergio, this was not your first take at Science, so maybe you're getting accustomed to being involved in something which is not part of your background as a cartoonist. Are you having second thoughts about it?

Sergio Ponchione I had previously been working on a chemistry-related comic book and yes, when we first talked about CECAM I felt a bit out of context. Moreover, the topic was somewhat

intimidating. But while becoming more involved, I also got more relaxed, thanks to the fantasy setting we opted for, which I like a lot. So, no second thoughts!

AP Giovanni, as a scriptwriter, how did you make your way through this step-by-step process – which is, very aptly, an approximation process – to find the right key for a story about the concept of simulation in science, and HPC?

GE In comics we can rely on both text and images, that's the main "pro". So, we had to use this medium to visually render how step-by-step approximation enables us to simulate complex processes.
The whole issue was to show how it was possibile to simulate reality with different levels of approximation, until simulation and reality are so close that they become one in some way, and what you get from the simulation is what you would get from reality.

RN When trying to communicate mathematics and modelling in particular, we often try to *tell* what our research's object is, and this is a mistake. If I simulate traffic flow and talk about it – not about the tools I am using to solve it – mathematics, modelling and simulation "disappear" behind the problem. And usually the application is not so important, because the same tools are used to solve very different problems, from biology to traffic flow.
The second remark is how mathematicians doing simulation speak about a "cartoon model", something which is not the real thing, and they know it. But in a way all science is a cartoon: a model is something that is simple, useful in order to understand phenomena, but it is in no way "real". It's something much simpler than reality and when the model can't describe some new situation, we change the model.

IP This was the core of what we wanted to convey. And it was very instructive to convey this message in comics form, which is a medium accessible to people in a broad range of ages. Given the very

nature of E-CAM, a European project, and CECAM, an institution devoted to the development of algorithms and furthering simulation in several fields, we wanted to keep a broad view of what we do. Finding the right language was our main effort, and it wasn't easy to keep our focus on the abstract process of thinking and developing models.

SB What we do at CECAM is multi-faceted and the temptation to try to say too much, sending out a confusing message, was always round the corner.
A first important thing is the higher level of abstraction, meaning that simple models still contain information: this is very clearly depicted in the story, where something always takes us one step closer to overcome the knight's specific challenge. On the other hand, things can go wrong and accidents happen: scientific processes are not linear.
Our story has different levels of interpretation and hopefully some of them will reach different people.

AP It should be remembered how Sergio has been publishing for years now in several countries. Moreover, he's particularly fond of the works of a few founding fathers of what modern comics are today, as a medium: great US cartoonists like Wally Wood, Jack Kirby, Steve Ditko and Will Eisner.
This said, Sergio, was *Ekham the Wise* inspired by any particular style?

SP Given its general tone, I had in mind the humor tradition of *Mad Magazine*, a classic US magazine featuring many great works by Wally Wood, for instance. I found it fitting. Then, as always, I tried to add something more personal: it's my way to have fun. The concept of different levels of definition gave me the opportunity to play with the page layout, as explained by Giovanni, from basic levels rendered by very simple linework, to the final levels with "higher resolution". I like playing with format, which is at the same time an important part of content: it shouldn't be just an exercise in style but go hand in hand with the subject matter, with the story.

GE I really liked your little monsters: the script's indication was simply "add monsters"... then I found a wholly new zoo of lovely little creepy creatures.

AP Sara, right before we started this conversation, you were telling us about how you were already getting some positive expert feedback about the story...

SB Well, I was having so much fun in the process of creating this story that I kept talking about it with my friends and people had to put up with me for a few months. There is this son of a very dear friend of mine, a 9-year-old boy who was eager to get to read the story, so I gave him the first draft as soon as it was available. Then I got this video call with him jumping on his bed, telling me very excitedly how much he had enjoyed the story, the witch, the knight, the little monsters (which he liked very much!)... we can safely say our first reader was very happy with what we did.

SP & GE Well, that's one of the greatest gratifications we can get from our work!

RN What is the age range you're trying to target with *Ekham the Wise*? The audience you aim to reach?

IP That was discussed at length since the very beginning. Our aim is to reach as broad as possible an audience, with a preference for teenagers and younger people with no specific interest in science. An audience we usually don't address, which isn't really reachable by the sort of events usually aimed for the general public. People who will go and attend a comic convention, Internet-savvy enough to find and download the comic book online, where it's going to be freely accessible.

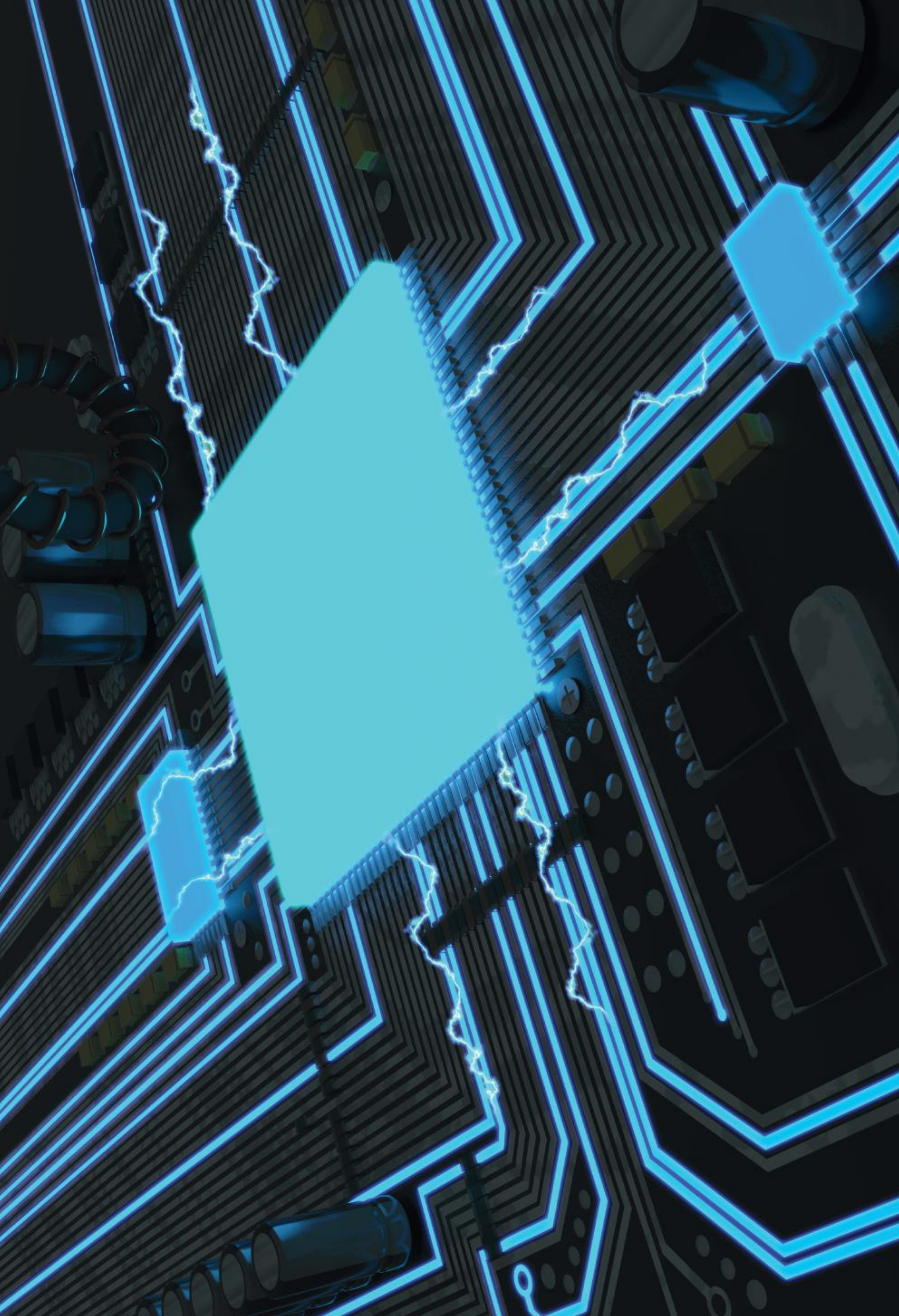
RN Young adults, or teenagers in secondary school, in the 13-25 range, are an interesting target because they find themselves trying to develop a taste for new things and like to be engaged.

IP That's why we thought this sort of comic book format might be attractive to them. Moreover, while nowadays so many people are exposed to computers and to science, the nature of modelling and computation isn't something so easily accessible and that was also part of our goal. Not even young people are fully aware of how it really works, how it has changed, and what engineering or project development is today.

GE That's one thing I wanted to stress, which I realized in the process of making this comic. A lot of things can be simulated, and when you don't have to test things in the "real world" huge amounts of time and resources are saved. Designing and running those big computers takes time and energy but nothing makes actual damage or endangers lives.

IP I would really like to stress how this has been a very interesting adventure for us: we learned a lot, in a very productive atmosphere. I will always remember the discussions we had at the beginning, trying to sort things out and to understand each other, so that we could explain what we were trying to do, and all our doubts! "Would the story of a knight be of any interest to a teenager nowadays?" we were asking ourselves. We had not done anything like this before. It all resulted in a very nice experience and we will keep on building on it, I'm sure.

SB I just wanted to add how interesting it was for me to learn how much skill and intelligence are hidden behind things that in the end want to be, or appear, simple. It is clearly something that we aspire to as scientists, because there is beauty in a simple explanation, but it was great to find the same kind of approach in what creative people like Giovanni and Sergio were doing with us.



Why are **experiment**, **theory**, *and* **simulation** *what today's scientists* **dream** *of being endowed with? Why is the latter so increasingly* **crucial** *for science? But first...*

What is a simulation?

CHRISTOPH DELLAGO

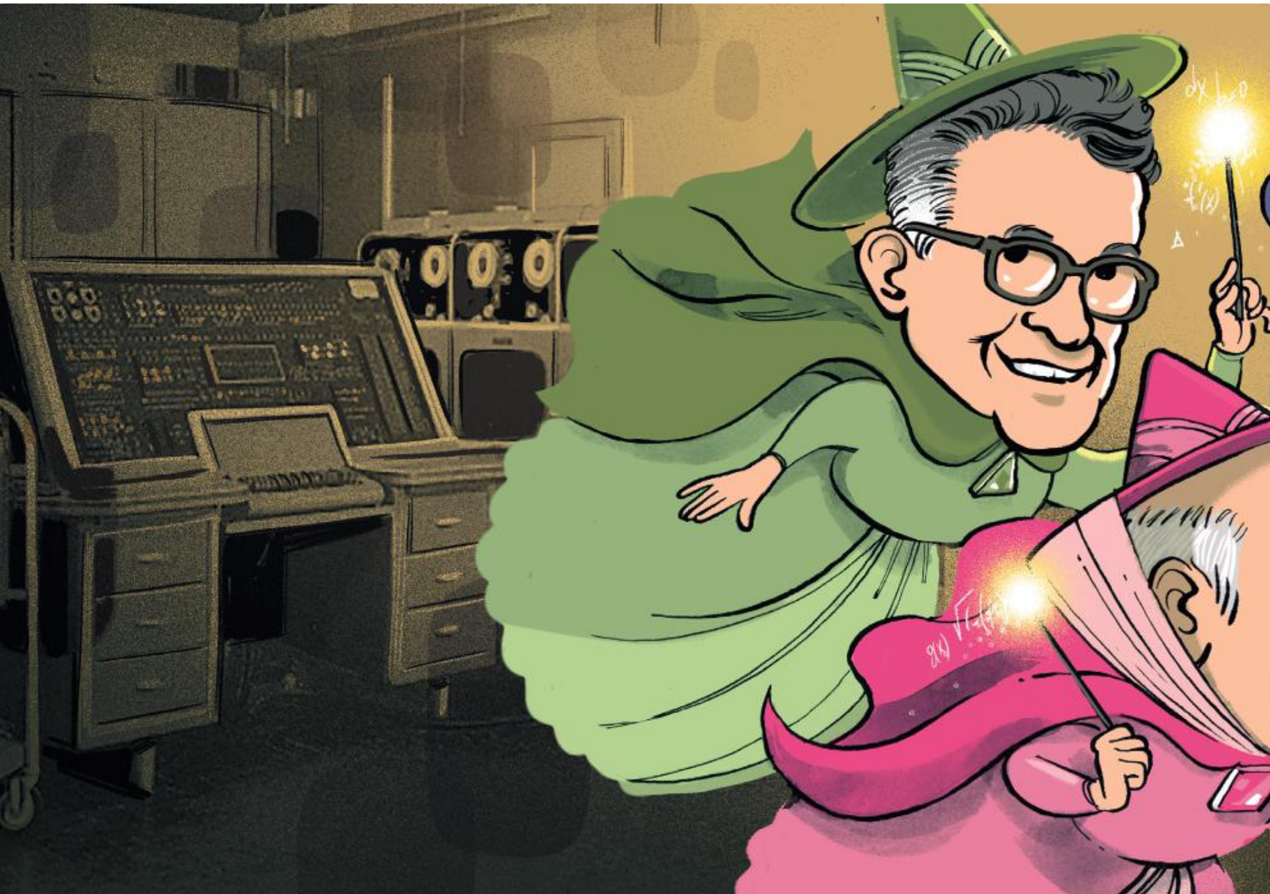
Why does water wet things? At first sight, this seems to be a childish question, but formulating this question properly and answering it based on the fundamental principles of physics is far from trivial. In fact, a true understanding of the properties of water and other everyday materials surrounding us has been achieved only recently through the use of powerful supercomputers. The quest to understand the world in which we live, however, began long before computers were available to carry out complicated calculations. Since the dawn of civilization, people have tried to make sense of the natural phenomena happening around them and recognizing patterns in a mostly chaotic world was often a matter of survival. For instance, early astronomers in ancient Mesopotamia attempted to understand regularities in the motion of celestial bodies, not only for religious reasons but also to predict tides and seasons. Since then, much progress has been made and today we have detailed knowledge and understanding of natural phenomena, ranging from the microscopic world of elementary particles to stars, galaxies and the entire universe. (Of course, many questions are still open and as the boundaries of our knowledge expand, also the white spots on the map of science become apparent.)
What are, then, the tools that have enabled the amazing progress of science from the early observations of the sun and the moon to the wonders of modern science that so deeply affect the way we live today? In the spirit of the *Ekham the Wise* fairy tale, we may imagine that once upon a time a child was born and the quest of this child was to become the first scientist and understand the world. As is customary in a fairy tale, three fairies come to celebrate the birth of the child and they bring gifts with them. The first and oldest fairy brings the

gift of experiment and tells the child: "By focusing on the measurable and excluding from your considerations all that is not measurable you will be able to obtain hard facts about nature. In your laboratory full of shiny (and expensive) gadgets you will make fantastic discoveries that will make you famous".

Fairy number two, middle aged and a bit disgruntled, brings the gift of theory and she says sternly: "By making everything as simple as possible (but not simpler), you will be able to construct approximate models of reality that capture the essential features of nature. Armed with your analytical mind, paper and pencil you will exploit the tools of mathematics to analyze your models and, if the conditions are propitious, you will even be able to solve them. Once in a while, you will be allowed a fleeting glimpse of the grand view, and you will be admired for your acumen."

The third and youngest fairy brings the gift of simulation. She cheerfully says to the child: "Don't worry about finding analytical solutions for simplified models. By using the powerful machines developed by our magicians, you will be able to study realistic models and get to the bottom of things. Furthermore, you will be able to study matter under conditions not accessible to experiments and make accurate predictions that will help us make tougher materials, develop new catalysts, fight diseases and predict the weather." Needless to say, provided with these gifts, the child grows up to be a talented scientist who finally frees the realm from the dragon of superstition, and all live happily ever after.

Computation has indeed developed into an incredibly powerful tool used in basically all areas of modern science. While computational approaches to solve problems predate the invention of digital computers and go back to Newton, Gauss and Jacobi, computational research took off in earnest after fast computing machines became available



in the late 1940s in the wake of the war efforts. Paralleling the development of faster computing hardware, scientists also developed new computational methods to exploit the capabilities of the computers. For instance, in the 1950s the newly developed Monte Carlo method based on random numbers made it possible, for the first time, to study realistic models of many-particle systems such as liquids and solids. At about the same time, the first molecular dynamics simulations were carried out, in which the trajectories of individual atoms are followed by solving the complicated mathematical equation that governs their motion. As a result of such a simulation, one can watch the complex dance of atoms as they collide with each other and study how the regular behavior of our macroscopic world emerges from this chaotic motion at the microscopic level. Since the first computer simulations were performed more than half a century ago, computation has deeply transformed the way science is done, opening new research directions. Today, increasingly realistic models of matter consisting of thousands or even millions of atoms and molecules can be investigated. For instance, with forces obtained from the basic principles of quantum mechanics, one can now carry out atomistic simulations to accurately predict the properties of materials that have not yet been made. Similarly, one can follow in detail the motion of a protein as it spontaneously folds into the structure required for its biological function. Computer simulations now play a crucial role in a wide range of fields, including physics, materials science chemistry and molecular biology. Thanks to the computer simulation, one can now answer the question "Why does water wet things?" and many others as well.

P.S. - Water wets things because the special bonds between its molecules make it stick!


Photo © Forschungszentrum Jülich/Ralf-Uwe Limbach

You can call it the **Holy Grail** of state-of-the-art scientific research. Power of Ten by Power of Ten, **High Performace Computing** has become the ultimate computer resource.

Giving computing a good name

GODEHARD SUTMANN

Computers play an important role in our daily lives and nearly everybody has a direct or indirect interaction with them: web surfing, text processing, watching videos, playing games or processing digital photo... These tools are accepted as common technological developments of our society. We take them for granted but often forget the enormous power, speed and complexity that are hidden behind electronic devices and which would not be possible without the pioneering work of computer scientists, software engineers and materials scientists. In fact, the technology routinely integrated into our smartphones or laptops has emerged as continuous development of cutting edge technology which has been driven by large scale computations, known as High Performance Computing (HPC). HPC is the tip of the arrow directing computer based development towards faster access of services and programs.

The evolution of computational resources over little more than the last 70 years is impressive. Standard computers, with which many of you are working nowadays, have computational power comparable to the biggest computer systems in the world 20 years ago. The trend observed so far is the doubling of processing power every 18 months. This has steadily led to an outstanding performance increase by a factor of x100 every 10 years. This behaviour, called Moore's law – after computer scientist Gordon Moore – has been stably observed until about 2010, when difficulties of power consumption and heat production started to pose new technical problems. A different avenue to further increase computer power was discovered via the so-called parallel computers, implementing the idea that union makes strength. By connecting processors, each executing specific tasks or subtasks, and allowing information exchange via a data network, the increase in power has accelerated quite remarkably. The first parallel computers were constructed in the 1970s and by applying this concept of multiplying the performance of computers by integrating more and faster processors, the performance of computers could be enhanced by a factor of x1000 every 10 years!

The power hidden inside the computer box cannot be easily visualised. Imagine a cup of dice being thrown each second. What would be the largest number of dice you would be able to sum up in one second without making errors or just estimating the result? Could you add five or six or even seven numbers? And how long would your concentration last to keep performing these summations reliably? The amount of operations (besides addition also multiplication) that a computer is able to process per second is a common measure for its performance. Compared to a computer, humans might feel very slow and clumsy. The first electronic computer was able to run at a performance of 500,000 operations per second (so called "flops": floating point operations per second)! If we think in terms of dice with an edge length of 1 cm, this would correspond to summing numbers on the faces of a straight line of connected dice of 5 km length, or an area of about 7x7 m^2, or a cube with a volume of about 0.8 m^3 – each second! Modern laptops or smartphones can handle billions of operations per second and use them to perform a number of tasks in parallel. This would correspond to summing the values of the faces of a straight line of dice 10,000 km long (a distance comparable to the earth's diameter)! Nowadays, the largest parallel computers in the world are even more advanced, performing more than a quadrillion operations per second ("1" followed by 15 zeros), which corresponds to a dice line of 10 billion km: more than 60 times the distance from Earth to Sun!

This amount of computational power reflects the complexity of the scientific challenge, which are overcome today, tackling problems of societal impact but also fundamental scientific questions, which increase our understanding of the world. Computers are used for weather forecasts, where complex mathematical models are solved on the basis of today's weather conditions in order to predict the weather for the coming days. Supercomputers are also often hidden behind products that we use on a daily basis. They contribute to the development of new materials with specific properties like low weight, low corrosion and high stability which are used for tools and devices. Pharmacological agents are tested or even discovered by computer simulations. Computer-based shape optimisations are commonly employed to produce planes with low air resistance and optimal flight properties, and

(a different kind of) optimisation is also used to improve performance of distribution in complex networks like the ones that bring electricity to our homes. Last but not least, simulation and modelling fully exploit high-end computers to expand our understanding of nature and look at phenomena ranging from systems at the atomic scale all the way up to geological formation or ecological systems.

Computer power will probably not be able to grow indefinitely due to material requirements, energy consumption and speed of information transmission between computer components. But scientists are optimistic about reaching the next stage, the so-called exaflop computing, within the next years. Exaflop computational power is very difficult to visualise and our example with dice is reaching its limits.

Imagine a number of operations per second of the order of a quintillion, "1" followed by 18 zeros! This corresponds to dice packed together and forming a block of linear length of 10 trillion km ("1" followed by 13 zeros, comparable to one light-year, i.e. about one quarter of the distance between the Earth and the Proxima Centauri star).

This is not only hard to imagine but also hard to accomplish. All components, including hardware, software, program design and algorithms (the smart recipes saying how to get to a solution) have to be developed in a concerted effort, which scientists call co-design.

Having only one optimised component is no longer sufficient to reach high quality and performance.

Imagine a perfectly constructed Formula One racing car: it will only be able to reach its highest performance if a super skilled pilot is driving, the streets allow for high speed and a team of experienced and specialised technicians is supporting with fuel, spare parts and smart ideas. It is a very similar situation with HPC and therefore the European Commission has set up programs where international teams work together with expertise coming from different fields: computer science, physics, chemistry, engineering, mathematics...

If and how computers will surpass exaflop computing is still an open question. New technologies, like quantum computing or neuromorphic computing are in different stages of development and are expected to contribute productively to the working environment of current supercomputers. The future might see a close combination of different sources for computing implemented in the so called modular supercomputing. We'll have to work, wait and see. In the meantime, let us appreciate the path travelled so far and enjoy the possibilities offered by current HPC resources. Human understanding goes well beyond the capacity to compute, but non-human computers can certainly be invaluable companions for our curiosity and imagination: it is up to us to put them to the best of uses!

Striving to put together
state-of-the-art **hardware**, **software**,
simulation-oriented **thinking**.
And **people**.

What is E-CAM?

IGNACIO PAGONABARRAGA
SARA BONELLA
ANA CATARINA MENDONÇA

E-CAM is a project funded by the European Union to support High Performance Computing (HPC) simulations and modelling in academia and industry. In simulation and modelling, software codes translate scientific ideas into a sequence of instructions, called algorithms, that can be executed by computers.
This translation must be faithful, so that accurate models of the real systems can be built, and must be efficient so that the codes are easy to execute for the computer and its calculating power can be fully harvested.
One of the main objectives of E-CAM is to ensure an optimal translation by bringing together the scientists that develop the algorithms and the software codes, and the scientific programmers, experts in software development and hardware, that optimise and implement them on top-of-the-line machines.
The close interactions within this interdisciplinary team deliver codes that can efficiently exploit existing and foreseeable computational resources. Respecting the collaborative spirit and public funding of the project, the E-CAM software is freely available to the community, under open copyright licences. Scientific ideas tested and understood via simulations run on computers - safe virtual environments, faster, and cheaper than laboratories - can then be further validated experimentally and eventually turned into solutions for important problems in our daily lives.
This alliance of theory and computation is very effective. Thanks to the combination of state-of-the-art scientific ideas and of efficient use of HPC, the E-CAM software enables, for example, to understand the action of new drugs or to build new green materials one

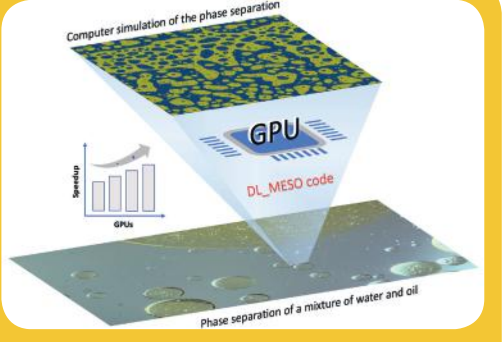
atom at a time. Such a broad and diverse range of applications requires equally broad and diverse scientific expertise. The unique characteristic of E-CAM is precisely to gather experts and foster collaboration not only among scientists and software engineers, but also between leading experts across four different key areas in simulation and modelling: classical molecular dynamics (modelling materials as collections of atoms that obey the laws of classical mechanics), electronic structure (which enables determination of the interactions between atoms from the more fundamental laws of quantum mechanics), quantum dynamics (where quantum mechanics is used to model how elements such as hydrogen behave or to describe the combined behaviour of nuclei and electrons), and meso- and multi-scale simulations (in which different length and time scales are bridged to study very large systems using coarse-grained models that bundle together sets of atoms that lose their specific identity without losing the relevant features of the system).

The E-CAM collaborative network builds on the long history of the Centre Européen de Calcul Atomique et Moléculaire (CECAM) that, for more than fifty years, has provided a focal point for simulation and modelling in Europe and beyond. CECAM coordinates the E-CAM project, bringing together researchers based in 10 European countries in a strong partnership that also includes 4 HPC centres belonging to the Partnership for Advanced Computing in Europe (PRACE) and the Hartree centre, at Daresbury Laboratory – a leading research infrastructure dedicated in particular to industrial computing. Importantly, E-CAM also has a portfolio of industrial partners and works with them on specific projects to foster the adoption of simulation and modelling as a valuable part of the production cycle in large conglomerates as well as in small and medium enterprises.

No progress can be sustained and furthered without competent and motivated human capital, so training on HPC oriented scientific applications is also a fundamental component of E-CAM. The project employs postdoctoral researchers in each of the four areas of simulation and modelling to work under the guidance of our leading scientists. Postdocs work closely with the scientific programmers to create highly efficient and scalable algorithms and codes. Some of the postdoctoral projects are developed in collaboration with our industrial partners, transferring skills from academia to industry and creating exciting career opportunities for our

CASE STUDY

MODELLING SURFACTANTS FOR PERSONAL CARE, HYGIENE, AND NUTRITION PRODUCTS.

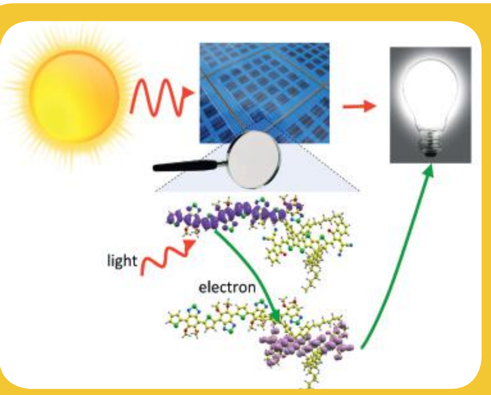


Surfactants are key ingredients in personal care products, dish soaps, laundry detergents, etc. At the microscopic level, they are very long chains of molecules, known as polymers. Controlling their properties, for example changing the atomic sequence or length of the chains, is a major industrial challenge for improving efficacy and sustainability of household products. Modelling of these systems is challenging due to their size (billions of atoms) and the environment in which they act. In collaboration with the Hartree center, E-CAM (thank you Michael Seaton and Jony Castagna!) has developed a highly efficient version of DL_MESO, a leading-edge code for simulating (also) surfactants. DL_MESO is routinely used by scientists in academia and by industries such as Unilever and IBM research UK.

young collaborators. More training is provided via workshops and schools. In particular, our Extended Software Development Workshops every year attract about 100 participants at different stages of their careers, from undergraduate students to senior researchers. These participants gain direct experience of modern software engineering techniques and open-source development tools to generate community codes. To facilitate access to training, lectures and lecture notes, exercise sessions, and useful reference material - both on scientific and on computer science topics - are collected and archived on the E-CAM on-line training portal. This growing repository of videos, slides, and prototypical codes is freely accessible to the broad community in simulation and modelling and will develop into a comprehensive web based training infrastructure complementing our in-person events. Dedicated training courses for industrial attendees are also organised, together with workshops providing access to the broad expertise of the E-CAM consortium. The potential benefits - economical and in terms of quality of the products delivered - of this approach are considerable, and our goal is to contribute to overcome the remaining technical, cultural and practical obstacles to its full exploitation. The multidisciplinary competence in E-CAM is key to react to diverse industrial

CASE STUDY

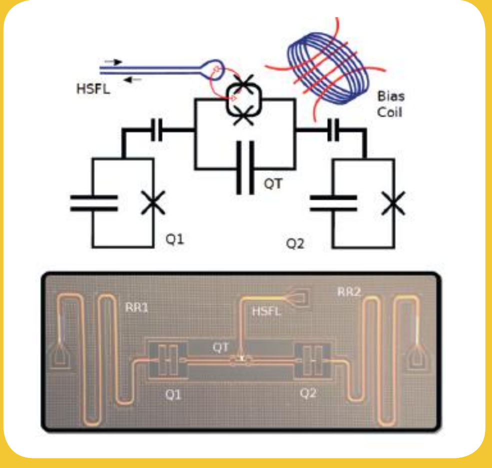
MODELLING ORGANIC SOLAR CELLS



Solar energy holds the promise of a renewable and sustainable alternative to fossil fuels. The creation of efficient, economical and non-polluting photovoltaic cells usable in large-area devices is a key challenge. In this collaboration with Merck E-CAM scientists (thank you David Lopez, Etienne Plésiat and Emilio Artacho!) used electronic structure calculations to study organic solar cells in which two molecules cooperate to convert sun energy into electric power. The mutual orientation of the molecules has paramount influence on efficiency. Our simulations quantified this influence, identified the preferred geometry of a specific pair of molecules and provided insight on relevant quantities characterising the overall performance of the cell.

CASE STUDY

MODELLING KEY COMPONENTS FOR QUANTUM COMPUTER PROTOTYPES



Quantum computers are fascinating candidates for a revolution in HPC, with the potential to increase computational power exponentially. While progress in their development is advancing, several scientific and technological challenges must be overcome to move beyond prototypes. In collaboration with an IBM Research team in Zürich led by Ivano Tavernelli, E-CAM (thank you Momir Mališ!) combined modelling and new software to study the logical gates controlling operations on the fundamental units carrying information (qubits). Simulations will help experimental work to build and control quantum gates more efficiently.

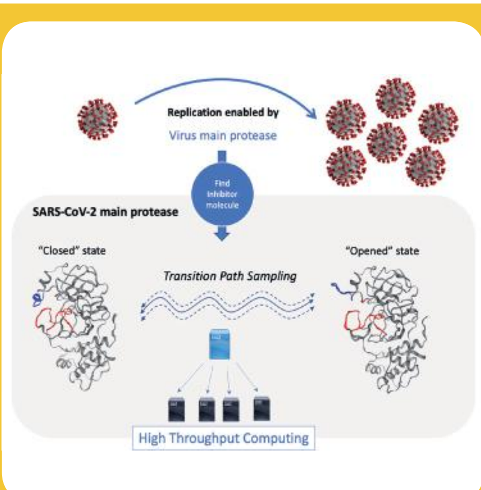
user's needs. Cutting-edge techniques and methods used in academic computational science usually take too long to transfer to industry, and conversely, interesting and significant problems and techniques driven by industrial applications are not efficiently communicated to the world of academic research. E-CAM addresses this gap by building communication channels between these two worlds.

The European Commission has funded fourteen more Centres of Excellence for Computing Applications and we are engaged in collaborations with our sister initiatives. We have developed projects with the MaX Centre for simulating materials at the exascale, the POP Centre on optimization and scaling of codes, the EoCoE centre for modelling of energy related topics, the CompBioMed Centre for Biomedical Applications and Focus CoE – a support initiative that promotes networking and actions useful for the Centres of Excellence. We also collaborate, in particular on training initiatives, with PRACE.

Through the actions described above, E-CAM makes an important contribution to the HPC ecosystem fostered by the European Commission. The scientific and technological developments of our project are fully integrated in the Horizon2020 programme and the EuroHPC joint undertaking, and would not be possible without this critical European financial contribution. These developments are enhanced by the commitment of all E-CAM team members to generate and disseminate high-quality scientific applications that, in synergy with other initiatives, will strengthen the European Research Area and, in time, contribute to improve our lives.

More information on E-CAM can be found at https://www.e-cam2020.eu/.

CASE STUDY
MODELLING PROTEINS VIA HTC



High Throughput Computing (or HTC) is the use of many computing resources over long periods of time, enabling the study of previously intractable systems. In E-CAM, HTC is used to study the SARS-CoV-2 main protease, responsible for the COVID-19 virus multiplication. A key difficulty in this problem is that the time scales involved are very long compared to those typically accessible via simulation. Advanced methods, co-developed by E-CAM scientists and known as Transition Path Sampling, were then adopted using the E-CAM-supported code OpenPathSampling (thank you Alan O'Cais and David Swenson!).

More than **half a century ago** a cutting-edge centre for scientific research started delivering **resources** and **know-how** to the science community. And it's active **today** more than ever.

What is CECAM?

IGNACIO PAGONABARRAGA
SARA BONELLA

The core mission of the Centre Européen de Calcul Atomique et Moléculaire (CECAM) is to promote fundamental research on advanced simulation and modelling and their application to frontier problems in science and technology. As the longest standing institution in this area, CECAM has been instrumental to establishing simulation and modelling as an innovative, effective and rich avenue of research and has fostered progress and collaboration in Europe and beyond. As stated by Carl Moser, CECAM's founder and first director, our philosophy is "to encourage a cooperative goal towards scientific development". Five generations of scientists separate the founding fathers of the field from the young scientists participating to our schools today, but this statement continues to describe the unique spirit of our activities.

Founded in 1969, CECAM was conceived from the start as a collaboration between scientists from different European countries. At its birth, it was funded by research institutions in France, the Netherlands, Belgium, and Italy. Today, 25 universities, national research centres, high performance computing centres and research institutes from 13 European countries and Israel sponsor its activities across a network of 17 nodes embedded in leading institutions of the European Research Area. The network is coordinated from the CECAM headquarters, hosted at the École Polytecnique Fédérale de Lausanne.

CECAM activities include the organisation of scientific workshops in emerging areas; advanced schools to train at the graduate and postdoctoral level; workshops on algorithmic and software development and exploitation; brain-storming and problem solving events on open challenges; the

development of collaborative research projects such as E-CAM; and the sponsorship of an international visitors and graduate training programme. In short, we welcome ideas from everybody interested in computational science and we strive to create the perfect environment for progress and exchange via active research and events. Every year, about 2,500 scientists at different stages of their careers – from leaders in the field to undergraduate students – take part in our activities across Europe, discuss and learn from each other.
The original focus of CECAM were atomistic and molecular simulations, applied to the physics and chemistry of condensed matter. During our first fifty years of service to the community, however, powerful advances in computer hardware and software have supported the extension of these methods to a wide range of problems in materials science, biology and medicinal chemistry. CECAM has always been very attentive to such developments and has helped to foster many of them. As the importance of simulation continues to grow in different emerging areas, CECAM has evolved its scope and structure to address these changes. For example, our communities are particularly interested in multiscale modelling of phenomena from a quantum to a constitutive equation description. CECAM also values and contributes to developing new statistical techniques that can extract relationships directly from data and data-driven initiatives, including machine learning and artificial intelligence.
With the continuing support of scientists in Europe and around the world, CECAM will keep identifying new, interesting directions in the domain of atomistic and materials modelling, inspire exciting activities and stimulate productive collaborations. Together, we shall endeavour to fulfil and enrich CECAM's mission and contribute to transmit its values to new generations of simulators.
You can discover more about CECAM at https://www.cecam.org/

A very **specific branch** of scientific research has been targeted as **crucial** and "**strategic**" by the **highest** European ranks. Here's the **hows** and the **whys**.

Vision of HPC and exascale from the European Commission

EUROPEAN COMMISSION

High Performance Computing (HPC), also known as supercomputing, refers to computing systems having extremely high computational capabilities.
These systems involve thousands of processors working in parallel to analyse billions of pieces of data in real time.
Today supercomputers are able to perform more than 10^{15} operations per second (petascale). Their next generation (exascale) will be performing one trillion (10^{18}) operations per second, a computing power level comparable to aggregating all computing capabilities of the cell phones of the entire population in the European Union. The first exascale supercomputers will be available around 2022.
HPC is today at the core of major advances and innovation and a strategic resource for Europe's future. It enables complex modelling and simulation but also extracting valuable knowledge from large amounts of data. HPC is used to solve scientific and engineering problems computationally so complex and demanding that simulations cannot be performed using general-purpose computers. The application areas range from cybersecurity, weather prediction, and molecular chemistry to energy exploration, and financial trading. In combination with Artificial Intelligence it has enormous potential to contribute to developing new treatments based on personalised medicine, reducing the time to market for innovative products or predicting and managing the effects of climate change.
In 2018, the European Commission established the European High Performance Computing Joint Undertaking. The EuroHPC Joint Undertaking aims at pooling EU and participating countries' resources to reach exascale capabilities and place a European supercomputer among the

world top five by 2021/2022. Today 32 European countries participate in this initiative. The development in Europe of this exascale supercomputing capability covering the whole value chain (from technology components to systems and machines, and to applications and skills) is crucial to support excellence research and boost innovation. It will also enable industrial sectors to become more productive and to scale up to higher value products and services by reducing product design and production cycles, accelerating the design of new materials, minimising costs, increasing resource efficiency and shortening and optimising decision processes.
European exascale capabilities will also benefit citizens by providing better understanding and responding to complex major societal challenges, such as environmental footprint of industry and society, or the impact of severe weather conditions. Finally, the development of this European value chain will underpin Europe's data sovereignty and scientific and industrial leadership. In 2019, the European Commission also selected 10 centres of excellence for HPC applications to support HPC scientific application in energy, climate, engineering, materials, optimisation, bio-molecular, environment, medicine and global challenges. The centres of excellence promote the use of upcoming exascale and extreme performance computing capabilities and scale up existing parallel codes towards exascale scaling performance. In addition, they address the skills gap in computational science in the targeted domains by specialized trainings for increased adoption of advanced HPC in industry and academia.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