

Ralf Deiterding

Curriculum Vitae

Contact Information

Title: Research & Development Associate
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Areas of research

Numerical analysis and scientific computing, hyperbolic problems, shock-capturing methods
Computational fluid dynamics, reactive and multiphase flows, fluid-structure interaction, shock and gas dynamics
Finite volume and discontinuous Galerkin schemes, adaptive mesh refinement and geometric multigrid methods, level set and embedded boundary methods
High performance parallel computing, object-oriented software frameworks

Education

Ph.D. in Applied and Computational Mathematics / Scientific Computing
Institute of Mathematics, Technical University Cottbus (Germany), Sep. 2003
Dissertation: *Parallel adaptive simulation of multi-dimensional detonation structures*, 280 pages
Advisor: G. Bader. Reporters: D. Kröner and U. Maas. Grade: “Summa cum laude”

Diploma in Applied and Technical Mathematics
Institute of Mathematics, Technical University Clausthal (Germany), Jan. 1998
Grade: “Very good”
Diploma thesis: *Numerical coupling of the 3D flow-code FIRE to the 1D hydraulic-code AMESIM for the design of Diesel-injection systems (in German)*. Advisor: H. J. Pesch

Professional experience

Research and Development Associate
Computer Science and Mathematics Division, Oak Ridge Nat. Lab., Sep. 06 - Present
Supervisor: E. F. d’Azevedo
Independent research on dynamically adaptive multiscale methods for simulating fluid-structure interaction events in cavitating and boiling cooling liquids at high pressures.

Senior Postdoctoral Scholar in Applied and Comp. Mathematics
California Institute of Technology, Aug. 04 - Jul. 06. Sponsor: D. I. Meiron
Chief software architect of the “Virtual Test Facility” software for simulating shock-driven fluid-structure interaction, ASC Alliance Center for Simulation of Dynamic Response of Materials

Postdoctoral Scholar in Applied and Computational Mathematics
California Institute of Technology, Jul. 03 - Jul. 04. Sponsor: D. I. Meiron

Research Assistant to G. Bader

Institute of Mathematics, Technical University Cottbus, Feb. 98 - Jun. 03

Project: *Analysis and simulation of flows for multi-component gas-mixtures*, supported by German DFG high-priority research program *Analysis and Numerics of Conservation Laws*

Teaching Assistant to G. Bader

Course *Efficient implementation of numerical algorithms in C*

Institute of Mathematics, Technical University Cottbus, Apr. 00 - Sep. 00

Honors and awards

Alston S. Householder Postdoctoral Fellowship in Scientific Computing for 2006

Best Ph.D. dissertation of Technical University Cottbus in 2003

Grant support

U.S. Department of Energy, Office of Science Postdoctoral Fellowship, Sep. 06 - Aug. 08

External consultant for Caltech ASC Alliance Center: Sep. 06 - Mar. 08

German Science Foundation grant Ba 840/3-3 (full position), Apr. 01 - Jun. 03

German Science Foundation grants Ba 840/3-1, Ba 840/3-2 (half position), Feb. 98 - Mar. 01

Publications

Journal papers

1. R. Deiterding. A parallel adaptive method for simulating shock-induced combustion with detailed chemical kinetics in complex domains, *Computers & Structures*, submitted.
2. R. Deiterding. Dynamically adaptive simulation of regular detonation structures using the Cartesian mesh refinement framework AMROC. *Int. Journal Computational Science and Engineering*, 2007, accepted and in press.
3. S. J. Laurence, R. Deiterding, H. G. Hornung. Proximal bodies in hypersonic flows. *J. Fluid Mech.* 590: 209–237, 2007.
4. R. Deiterding, F. Cirak, S. P. Mauch, D. I. Meiron. A virtual test facility for simulating detonation- and shock-induced deformation and fracture of thin flexible shells. *Int. J. Multiscale Computational Engineering* 5(1): 47–63, 2007.
5. C. Pantano, R. Deiterding, D. J. Hill, D. I. Pullin. A low-numerical dissipation patch-based adaptive mesh refinement method for large-eddy simulation of compressible flows, *J. Comp. Physics* 221 (1): 63–87, 2007.
6. F. Cirak, R. Deiterding, S. P. Mauch. Large-scale fluid-structure interaction simulation of viscoplastic and fracturing thin shells subjected to shocks and detonations. *Computers & Structures* 85 (11-14): 1049–1065, 2006.
7. R. Deiterding, R. Radovitzky, S. P. Mauch, L. Noels, J. C. Cummings, D. I. Meiron. A Virtual Test Facility for the efficient simulation of solid materials under high energy shock-wave loading, *Engineering with Computers* 22 (3-4): 325–347, 2006.

Book chapters

1. R. Deiterding and G. Bader. High-resolution simulation of detonations with detailed chemistry. In G. Warnecke, editor, *Analysis and Numerics of Conservation Laws*, pages 69–91, Springer, Berlin, 2005
2. R. Deiterding. Detonation Simulation with the AMROC Framework. In K. Kremer and V. Macho, editors, *Forschung und wissenschaftliches Rechnen: Beiträge zum Heinz-Billing-Preis 2003*, pages 63–77, Ges. für Wiss. Datenverarbeitung, Göttingen, 2004.

Refereed proceedings

1. M. Lombardini, R. Deiterding, D. I. Pullin. Large-eddy simulation of the Richtmyer-Meshkov instability in a converging geometry. In J. Meyers et al., editors, *Quality and Reliability of Large-Eddy Simulations, Proc. of QLES 2007 Int. Symposium, Leuven*, pages 283–294, Ercoftac Series, Vol. 12, Springer, Netherlands, 2008.
2. S. Browne, Z. Liang, R. Deiterding, J. E. Shepherd. Detonation front structure and the competition for radicals. *Proc. of the Combustion Institute* 31(2): 2445–2453, 2007.
3. C. Pantano, R. Deiterding, D. J. Hill, D. I. Pullin. A low-numerical dissipation patch-based, adaptive mesh refinement method for large-eddy simulation of compressible flows. In S. Kassinos, P. Moin, editors, *Complex Effects in Large Eddy Simulation, Proc. of LES 2005 Int. Symposium, Cyprus*, pages 251–262, Lecture Notes in Computational Science and Engineering, Vol. 56, Springer, New York, 2007.
4. R. Deiterding, F. Cirak, S. P. Mauch, D. I. Meiron. A virtual test facility for simulating detonation-induced fracture of thin flexible shells. In V. N. Alexandrov et al., editors, *6th Int. Conf. Computational Science*, pages 122–130, Lecture Notes in Computer Science 3992, Springer, Berlin, 2006.
5. R. Deiterding. A high-resolution method for realistic detonation structure simulation. In W. Takahashi, T. Tanaka, editors, *Proc. Tenth International Conference on Hyperbolic Problems: Theory, Numerics, Applications*, Sep 13-17, 2004, Vol. 1, pages 343–350, Yokohama Publishers, 2006.
6. R. Deiterding. An adaptive Cartesian detonation solver for fluid-structure interaction simulation on distributed memory computers. In A. Deane et al., editors, *Parallel Computational Fluid Dynamics - Theory and Application, Proc. Parallel CFD 2005 Conference*, pages 333–340, Elsevier, 2006.
7. R. Deiterding. Detonation structure simulation with AMROC. In L. T. Yang et al., editors, *High Performance Computing and Communications 2005*, pages 916–927, Lecture Notes in Computer Science 3726, Springer, Berlin, 2005.
8. R. Deiterding. Construction and application of an AMR algorithm for distributed memory computers. In T. Plewa et al., editors, *Adaptive Mesh Refinement - Theory and Applications, Proc. of the Chicago Workshop on Adaptive Mesh Refinement Methods*, Sep. 2003, pages 361–372, Lecture Notes in Computational Science and Engineering, Vol. 41, Springer, New York, 2005.
9. R. Deiterding. Efficient simulation of multi-dimensional detonation phenomena. In A. Handlikova et al, editors, *Proc. of ALGORITMY 2002, 16th Conf. on Scientific Computing*, pages 94–101. Dep. of Math. and Descriptive Geometry, Slovak Univ. of Techn., Bratislava, Slovakia.

Other proceedings

1. R. Deiterding. Adaptive high-resolution simulation of realistic gaseous detonation waves. *Proc. Appl. Math. Mech.* Special Issue: 6th Int. Congress on Industrial and Applied Mathematics (ICIAM07), Zürich 2007, 2 pages, in press.
2. R. Deiterding. An adaptive level set method for shock-driven fluid-structure interaction. *Proc. Appl. Math. Mech.* 7(1): 2100037–2100038, 2007. Special Issue: 6th Int. Congress on Industrial and Applied Mathematics (ICIAM07), Zürich 2007.
3. R. Deiterding. Numerical simulation of transient detonation structures in $H_2 - O_2$ mixtures in smooth pipe bends. In P. Bauer et al., editors, *21st Int. Colloquium on the Dynamics of Explosions and Reactive Systems*, Poitiers, Jul. 2007, CD-ROM, 4 pages.
4. R. Deiterding, F. Cirak, S. P. Mauch, D. I. Meiron. A virtual test facility for simulating detonation-induced deformation and fracture of thin flexible shells. In P. Wesseling et al., editors, *European Conference on Computational Fluid Dynamics 2006*, Egmond aan Zee, Sep. 2006, CD-ROM, 18 pages.
5. C. Pantano, R. Deiterding, D. J. Hill, D. I. Pullin. A low-numerical dissipation patch-based, adaptive mesh refinement method for large-eddy simulation of compressible flows. *Journal of Physics: Conference Series* 46 (2006) 48–52. *Proc. of SciDAC 2006*.
6. R. Deiterding. Numerical structure analysis of regular hydrogen-oxygen detonations. In *Proc. of Fall Meeting of Western States Section of the Combustion Institute*, Los Angeles, Oct. 2003, CD-ROM, 24 pages.
7. R. Deiterding. Accurate simulation of Rayleigh-Taylor instabilities. In P. Jonas and V. Uruba, editors, *Proc. of Colloquium on Fluid Dynamics*, Prague, Oct. 1999, pages 37–44.
8. G. Bader, R. Deiterding. A distributed memory adaptive mesh refinement package for inviscid flow simulations. In P. Jonas and V. Uruba, editors, *Proc. of Colloquium on Fluid Dynamics*, Prague, Oct. 1999, pages 9–14.

Technical reports

1. J. Steensland, J. Ray, H. Johansson, R. Deiterding. An improved bi-level algorithm for partitioning dynamic grid hierarchies. SAND2006-2487. Sandia National Laboratories, May 2006, 36 pages.
2. C. Pantano, R. Deiterding, D. J. Hill, D. I. Pullin. A low-numerical dissipation patch-based adaptive mesh refinement method for large-eddy simulation of compressible flows. CIT-ASCI-TR319. California Institute of Technology, Sep. 2005, 49 pages.
3. Simulation of thermal ignition of an ozone-oxygen mixture in a cylindrical vessel. NMWR-00-4, Technical University Cottbus, Nov. 2000, 11 pages.
4. Simulation of a shock tube experiment with non-equilibrium chemistry. NMWR-00-3, Technical University Cottbus, Oct. 2000, 12 pages.

Meetings and symposia

Invited talks

1. Adaptive finite volume methods for simulating multidimensional gaseous detonation waves, Minisymposium on Computational Challenges on Modeling Transient Detonation, *61st Annual American Physical Society Division of Fluid Dynamics Meeting*, San Antonio, Nov. 23 - 25, 2008.

2. Fluid-structure interaction simulation of shock wave impact on solid structures, keynote lecture in Minisymposium on Recent Advances in Numerical Methods for Hyperbolic Problems, *8th World Congress on Computational Mechanics*, Venice (Italy), Jul. 2, 2008.
3. Accurate simulation of transient cellular structures in gaseous detonations with an adaptive high-resolution method, Minisymposium on Adaptive Numerical Methods for Combustion Simulation, *12th Int. SIAM Conference on Numerical Combustion*, Monterey, Mar. 31, 2008.
4. A parallel SAMR framework for strongly driven fluid-structure interaction problems, Minisymposium on Structured Adaptive Mesh Refinement (SAMR) on Supercomputers, *6th SIAM Conf. on Parallel Data Processing*, Atlanta, Mar. 13, 2008.
5. Numerical simulation of realistic detonation structures, Minisymposium on Numerical Methods for Chemically Reacting Flows, *6th Int. Congress on Industrial and Applied Mathematics*, Zürich (Switzerland), Jul. 19, 2007.
6. AMROC - A Cartesian SAMR framework for compressible gas dynamics, Minisymposium on Integrated Software Frameworks for Advanced Scientific and Engineering Applications, *SIAM Conference on Computational Science and Engineering*, Costa Mesa, Feb. 22, 2007.
7. Simulation of supersonic combustion phenomena in evolving geometries with Cartesian upwind methods, Minisymposium on Wave Propagation Algorithms for Complex Applications, *SIAM Conference on Computational Science and Engineering*, Costa Mesa, Feb. 21, 2007.
8. A dynamically adaptive high - resolution method for detonation simulation, Minisymposium on Recent Advances in Fixed-grid Numerical Methods for Hyperbolic Problems, *7th World Congress on Computational Mechanics*, Los Angeles, Jul. 21, 2006.
9. Coupled simulation of detonation-induced fracture of thin flexible shells, Minisymposium on Methods and Applications in Coupled Engineering Simulation, *7th World Congress on Computational Mechanics*, Los Angeles, Jul. 16, 2006.
10. Adaptive simulation of cellular detonation structures in low-pressure hydrogen-oxygen mixtures under transient conditions, Minisymposium on Flow Simulations and Algorithms on Block-structured Adaptively Refined Meshes, *Eleventh Int. SIAM Conference on Numerical Combustion*, Granada (Spain), Apr. 24, 2006.
11. The Virtual Test Facility – A multi-physics framework for simulating the dynamic response of materials. Minisymposium on Infrastructures for Developing Large Scale and Dynamic Computational Mechanics Applications, *Eighth U.S. National Congress on Computational Mechanics*, Austin, Jul. 25, 2005.
12. Dynamic mesh adaptation in detonation-driven fluid-structure problems, Minisymposium on Error Control and Mesh Adaptation in FEA, *Third MIT Conference on Computational Fluid and Solid Mechanics*, Boston, Jun. 14, 2005.

Contributed talks

1. Efficient fluid-structure interaction simulation of plates subjected to underwater shock loading, *Int. Workshop on Fluid-Structure Interaction: Theory, Numerics and Applications*, Herrsching (Germany), Sep. 29 - Oct. 1, 2008.
2. Numerical simulation of transient detonation structures in $H_2 - O_2$ mixtures in smooth pipe bends, *21st Int. Colloquium on the Dynamics of Explosions and Reactive Systems*, Poitiers (France), Jul. 23, 2007.

3. Large-scale simulation of shock- and detonation-driven fluid-structure interaction phenomena. *6th Int. Congress on Industrial and Applied Mathematics*, Zürich, Jul. 19, 2007.
4. Large-scale fluid-structure interaction simulation of viscoplastic and fracturing thin shells subjected to shocks and detonations. *4th M.I.T. Conference on Computational Fluid and Solid Mechanics*, Boston, Jun. 14, 2007.
5. A Cartesian structured AMR framework for parallel fluid-structure interaction simulation. *Int. Conf. Parallel Computational Fluid Dynamics*, Busan (South Korea), May 16, 2006.
6. A Cartesian structured AMR framework for parallel fluid-structure interaction simulation. *5th SIAM Conf. on Parallel Data Processing*, San Francisco, Feb. 22, 2006.
7. AMROC - A Cartesian structured AMR framework for distributed memory computers. *Int. Conf. Parallel Computational Fluid Dynamics*, Maryland, May 25, 2005.
8. Detonation structure simulation with AMROC. *High Performance Computing and Communications 2005*, Sorrento (Italy), Sep. 23, 2005.
9. Towards simulation of detonation-induced thin-shell dynamics with the Virtual Test Facility. *3rd Workshop on Comp. Methods for Multidimensional Reactive Flows*, Heidelberg (Germany), Jan. 27, 2005.
10. High-resolution simulation of realistic detonation structures. *Tenth International Conference on Hyperbolic Problems: Theory, Numerics, Applications*, Osaka (Japan), Sep. 14, 2004.
11. Numerical structure analysis of regular hydrogen-oxygen detonations. *Fall Meeting of Western States Section of the Combustion Institute*, Los Angeles, Oct. 2003.
12. Construction and application of an AMR algorithm for distributed memory computers. *Chicago Workshop on Adaptive Mesh Refinement Methods*, Sep. 4, 2003,
13. Numerical simulation of cellular detonation structure. *2nd Workshop on Comp. Methods for Multidimensional Reactive Flows*, Heidelberg, Dec. 2002.
14. Numerical simulation of cellular detonation structures in detonations, *6th Workshop on Conservation Laws*, Hirschegg (Austria), Sep. 2002.
15. Efficient simulation of multi-dimensional detonation phenomena. *ALGORITMY 2002, 16th Conf. on Scientific Computing*, Podbanske (Slovakia), Sep. 2002.
16. Accurate simulation of detonation phenomena. *ANumE-Colloquium*, Freiburg, Feb. 2002.
17. An AMR-algorithm for distributed memory computers. *11th GAMM-Workshop on Numerical Methods in Fluid Mechanics*, Kirchzarten (Germany), Nov. 26, 2001.
18. Adaptive high resolution methods for inviscid flow problems with chemical reaction. *Workshop on Computational Methods for Multidimensional Reactive Flows*, Heidelberg, Sep. 2000.
19. Accurate simulation of Rayleigh-Taylor instabilities. *Proc. of Colloquium on Fluid Dynamics*, Prague (Czech Republic), Oct. 1999.
20. Adaptive simulation of inviscid gas-flows on super-computers (in German), *South-east German Colloquium on Numerical Mathematics*, Freiberg, Apr. 23, 1999.

Organized

1. Minisymposium on Recent Advances in Numerical Methods for Hyperbolic Problems, *8th World Congress on Computational Mechanics*, Venice (Italy), Jul. 2 - 3, 2008 (with S. Karabasov, V. Goloviznin, T. Kozubskaya, Yoko Takakura, and M. Lukakova).

2. Minisymposium on Adaptive Numerical Methods for Combustion Simulation, *12th Int. SIAM Conference on Numerical Combustion*, Monterey, Mar. 31 - Apr. 1, 2008 (with J. Banks).
3. Minisymposium on Structured Adaptive Mesh Refinement (SAMR) on Supercomputers, *6th SIAM Conf. on Parallel Data Processing*, Atlanta, Mar. 13, 2008.

Selected posters

1. A Cartesian AMR framework for detonation- and shock-driven fluid-structure interaction simulation. DOE Office Office of Advanced Scientific Computing Research Applied Mathematics PI Meeting, Lawrence Livermore National Laboratory, May 24, 2007.
2. Accurate simulation of detonation phenomena. *Int. Conf. Dynamic Days 2002*, Heidelberg, Jul. 15-17, 2002.
3. Object-oriented design of an AMR-algorithm for distributed memory computers. *8th Int. Conf. on Hyperbolic Problems*, Magdeburg (Germany), Feb. 2000.

Seminars and colloquia

1. Embedded boundary finite volume methods for simulating shock-driven fluid-structure interaction, *Seminar for Applied Mathematics, University of Kiel*, Jul. 9, 2008.
2. A framework for parallel adaptive Cartesian finite volume methods in evolving geometry, *Oak Ridge National Laboratory*, Apr. 17, 2006.
3. Application of adaptive Cartesian finite volume upwind schemes for hyperbolic computational fluid dynamics and fluid-structure coupling, *Center for Computational Engineering Science, RWTH Aachen (Germany)*, Apr. 3, 2006.
4. A parallel adaptive ghost-fluid method for hyperbolic computational fluid dynamics and fluid-structure coupling, *Institute for Applied Mathematics, University Freiburg (Germany)*, Mar. 28, 2006.
5. Application of Cartesian SAMR for real-world CFD, *Center for Computation and Technology, Louisiana State University Baton Rouge*, Mar. 20, 2006.
6. Structured adaptive mesh refinement in the Virtual Test Facility, *Center for Risk Studies and Safety, University of California Santa Barbara*, Mar. 6, 2006.
7. Application of Cartesian finite volume upwind schemes for real-world CFD, *Centre for Analysis, Scientific computing and Applications, Technical University Eindhoven (Netherlands)*, Nov. 25, 2005.
8. Adaptive multilevel discretizations for computational fluid dynamics, Graduate Aeronautical Laboratories, *California Institute of Technology, Pasadena*, Apr. 02, 2004.
9. Simulation of real detonation and turbulence phenomena in compressible gaseous flows with self-adaptive finite volume methods (in German), *Technical University Cottbus*, Jan. 2004.
10. Adaptive simulation of multi-dimensional structures (in German), *Institute for Applied Mathematics, University Freiburg*, Jun. 03, 2003.
11. Adaptive finite volume methods for detonation simulation, Center of Advanced Computational Research, *Californian Institute of Technology, Pasadena*, May 20, 2003.
12. Application of parallel adaptive mesh refinement for detonation structure simulation, *Rutgers University, Piscataway*, Feb. 19, 2003.

- Adaptive simulation of unstable detonation phenomena, *Seminar of Applied Mathematics, ETH Zürich*, May 5, 2002.

Software

Virtual Test Facility for simulating the dynamic response of materials

<http://www.cacr.caltech.edu/asc>

430,000 lines of code C++, C, Fortran 77, Fortran 90, ~ 27 % (largest contribution) of program text by R. Deiterding

AMROC - Adaptive Mesh Refinement in Object-oriented C++

<http://amroc.sourceforge.net>

140,000 lines of code C++, C, Fortran 77, ~ 75 % of overall program text by R. Deiterding

Teaching

Courses

Devised, implemented and supervised lab exercises for course *Efficient implementation of numerical algorithms in C*, Technical University Cottbus, Apr. 00 - Sep. 00

Student supervision

DOE Computational Science Graduate Fellow internship of J. Ziegler, *Direct numerical simulation of the Mach reflection phenomenon in gaseous detonation waves*, 2008

Graduate student summer internship of V. Srikrishnan, *Computational methods for implicit geometry representation*, 2007

Summer undergraduate research fellowship of R. Rotta, *Efficient parallelization strategies for hierarchical AMR algorithms*, 2005

Summer undergraduate research fellowship of R. Rotta, *Load-balancing strategies for parallel AMR algorithms*, 2004

Diploma thesis of M. Hausdorf, *Realization of adaptive multigrid methods for finite difference and finite volume discretization (in German)*, Jul. 2002 - Jan. 2003

Undergraduate research project of M. Enculescu, *Numerical simulation of one-dimensional ZND detonations (in German)*, 2001

Several ancillary student projects in computational fluid dynamics, numerical methods for hyperbolic conservation laws, scientific visualization, 1999 - Jun. 2003

Student advising

J. Krimmel, graduate student of T. Colonius (Mechanical Engineering Caltech), numerical simulation of shock wave lithotripsy, Jun. 2005 - Present

M. Lombardini, graduate student of D. I. Pullin (Graduate Aeronautical Laboratory Caltech), adaptive large-eddy simulation of shock-driven compressible turbulence, Dec. 2004 - Present

S. Laurence, graduate student of H. G. Hornung (Graduate Aeronautical Laboratory Caltech), numerical simulation of bodies in hypersonic flow, Jun. 2004 - Aug. 2006

C. Mouton, graduate student of H. G. Hornung, numerical simulation of three-dimensional Mach reflection phenomena, 2005

G. K. O'Reilly, graduate student of D. I. Pullin, numerical simulation of shock-vortex interaction, 2004

A. Rohde, graduate student of M. Mutz (Environmental Sciences Techn. Univ. Cottbus), simulation of porous media flow in sediment layers, 1999

Professional activities

Referee

Progress in Computational Fluid Dynamics
Proc. of the Royal Soc. Series A
Int. J. for Numerical Methods in Fluids
Computers & Structures
Engineering with Computers
Int. Parallel and Distributed Processing Symposium 2005
Eurographics 2004

Affiliations

Member of Society for Industrial and Applied Mathematics (SIAM)
Member of Association for Computing Machinery (ACM)
Member of the American Physical Society

Specific skills

Programming languages: C++, C, Fortran 77, Fortran 90, Pascal, Modula, Python, Basic

Parallel libraries: MPI, OpenMP

Parallel system experience: Various Linux Beowulf clusters, IBM SP2 - SP5, Compaq Q, Sun and IBM SMP systems

Scientific visualization: IBM DataExplorer, Paraview, VisIt, Visual 3

Mathematical software: Matlab, Mathematica, Maple

Languages

German: native speaker

English: fluent, written and spoken

French: intermediate

Russian: basic

References

1. Daniel I. Meiron
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3. Dale Pullin
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