Stanford

Eric Darve

Director, Institute for Computational and Mathematical Engineering (ICME) and Professor of Mechanical Engineering

CONTACT INFORMATION

- **Administrator**

  Michelle Taylor - Administrative Associate

  Email mtaylor9@stanford.edu

  Tel (650) 723-3610

Bio

BIO

The research interests of Professor Darve span across several domains, including machine learning for science and engineering, large-language models, transformer models, surrogate and reduced order modeling, stochastic inversing, anomaly detection, numerical linear algebra, high-performance, parallel, and GPU computing.

Professor Darve received his Ph.D. in Applied Mathematics at the Jacques-Louis Lions Laboratory in the Pierre et Marie Curie University, Paris, France. His advisor was Prof. Olivier Pironneau, and his Ph.D. thesis was entitled "Fast Multipole Methods for Integral Equations in Acoustics and Electromagnetics." He was previously a student at the Ecole Normale Supérieure, rue d'Ulm, Paris, in Mathematics and Computer Science.

Prof. Darve became a postdoctoral scholar with Profs. Moin and Pohorille at Stanford and NASA Ames in 1999 and joined the faculty at Stanford University in 2001. He is a member of the Institute for Computational and Mathematical Engineering.

Prof. Darve has received many awards, including the H. Julian Allen Award, NASA (2010), the Habilitation à Diriger des Recherches, France (2007), the Leslie Fox Prize in Numerical Analysis, IMA (2001), and the James H. Clark Faculty Scholar, Stanford University (2001).

ACADEMIC APPOINTMENTS

- Professor, Mechanical Engineering
- Member, Bio-X
- Member, Institute for Computational and Mathematical Engineering (ICME)

ADMINISTRATIVE APPOINTMENTS

- Director, Institute for Computational and Mathematical Engineering (ICME), (2024-2029)

HONORS AND AWARDS

- Kenneth and Barbara Oshman Faculty Scholar Award, Stanford University (2011)

- H. Julian Allen Award, NASA (2010)
- Habilitation à Diriger des Recherches, France (2007)
- Leslie Fox Prize in Numerical Analysis, IMA (2001)
- James H. Clark Faculty Scholar, Stanford University (2001)

BOARDS, ADVISORY COMMITTEES, PROFESSIONAL ORGANIZATIONS

- Associate Editor, SIAM Journal on Scientific Computing (SISC) (2014 - present)
- Associate Editor, Journal of Computational Physics (JCOMP) (2013 - 2024)

PROFESSIONAL EDUCATION

- PhD, Paris VI University, Paris , Applied Mathematics (1999)
- MS, Paris IX University, Paris , Applied Mathematics (1994)
- BS, Paris VI University, Paris , Mathematics and Physics (1993)

PATENTS

- Daniel Ratner, Eric Felix Darve, Ryan Humble. "United States Patent US20230409422A1 Systems and Methods for Anomaly Detection in Multi-Modal Data Streams", Leland Stanford Junior University, Jun 20, 2023
- Ziyi Yang, Eric Felix Darve, Iman Soltani Bozchalooi. "United States Patent US20200410285A1 Anomaly Augmented Generative Adversarial Network", Ford Global Technologies LLC Leland Stanford Junior University, Jun 25, 2020

LINKS

- https://me.stanford.edu/people/eric-darve: https://me.stanford.edu/people/eric-darve

Research & Scholarship

CURRENT RESEARCH AND SCHOLARLY INTERESTS

Professor Darve's research work emphasizes the development of numerical methods for machine learning in science and engineering applications, large-language models, anomaly detection, numerical linear algebra, fast algorithms, high-performance scientific computing, and parallel computing. In various engineering scenarios, the computational cost of simulating intricate and large systems is considerable and frequently exceeds the present computer capabilities. Therefore, the Darve research group is working on innovative numerical strategies to lower this computational cost and facilitate the simulation of complex systems over realistic timescales.

Keywords: large-language models, transformer models, numerical linear algebra (fast linear solvers, fast QR factorization, eigenvalue solvers, applications in geoscience and electric power grid), physics-informed machine learning (inverse modeling using PhysML, auto-encoders, GAN for uncertainty in predictive and inverse modeling, Kriging and statistical inversing, applications in geoscience, fluid mechanics and computational mechanics), anomaly detection (GAN-based algorithms, self-supervised machine learning, applications with the SLAC National Accelerator Laboratory), reinforcement learning for engineering applications.

Teaching

COURSES

2025-26

- First Year Seminar Series: CME 300 (Aut)
- Introduction to parallel computing using MPI, openMP, and CUDA: CME 213, ME 339 (Spr)
- Numerical Linear Algebra: CME 302 (Aut)

2024-25

- First Year Seminar Series: CME 300 (Aut)
- Introduction to parallel computing using MPI, openMP, and CUDA: CME 213, ME 339 (Spr)
- Numerical Linear Algebra: CME 302 (Aut)

2023-24

- Introduction to parallel computing using MPI, openMP, and CUDA: CME 213, ME 339 (Spr)
- Numerical Linear Algebra: CME 302 (Aut)
- Ordinary Differential Equations for Engineers: CME 102, ENGR 155A (Win)

2022-23

- Introduction to parallel computing using MPI, openMP, and CUDA: CME 213, ME 339 (Spr)
- Machine Learning for Computational Engineering.: CME 216, ME 343 (Win)
- Numerical Linear Algebra: CME 302 (Aut)

STANFORD ADVISEES

Orals Chair

Faisal As'ad

Doctoral Dissertation Advisor (AC)

Junlin Luo, John Winnicki

Doctoral Dissertation Co-Advisor (AC)

Luc Houriez, Bryan Hwang, Natalia Rubio, Apoorv Srivastava, Elise Yang

Master's Program Advisor

Himansu Pathak, Sukeerth Ramkumar, Chenhao Zhu

Doctoral (Program)

Shai Bernard, Larry Marshall

Publications

PUBLICATIONS

- **Bi-fidelity interpolative decomposition for multimodal data** *COMPUTER METHODS IN APPLIED MECHANICS AND ENGINEERING*
  Cutforth, M., Fan, T., Zahtila, T., Doostan, A., Darve, E.
  2026; 451
- **Data-driven bifurcation handling in physics-based reduced-order vascular hemodynamic models.** *Computer methods and programs in biomedicine*
  Rubio, N. L., Darve, E. F., Marsden, A. L.
  2025; 276: 109230
- **Coincident learning for beam-based rf station fault identification using phase information at the SLAC linac coherent light source** *PHYSICAL REVIEW ACCELERATORS AND BEAMS*
  Liang, J., Colocho, W., Decker, F., Humble, R., Morris, B., O'Shea, F. H., Steele, D. A., Zhang, Z., Darve, E., Ratner, D.
  2025; 28 (12)
- **Reinforced ridges in Thwaites Glacier yield insights into resolution requirements for coupled ice sheet and solid Earth models** *CRYOSPHERE*
  Houriez, L., Larour, E., Caron, L., Schlegel, N., Adhikari, S., Ivins, E., Pelle, T., Seroussi, H., Darve, E., Fischer, M.

2025; 19 (10): 4355-4372

- **Transfer Learning for Anomaly Detection in Rotating Machinery Using Data-Driven Key Order Estimation** *IEEE TRANSACTIONS ON AUTOMATION SCIENCE AND ENGINEERING*
  Liang, J., Shui, H., Gupta, R., Upadhyay, D., Darve, E.
  2025; 22: 13310-13326
- **Physically Interpretable Representation and Controlled Generation for Turbulence Data**
  Fan, T., Cutforth, M., D'Elia, M., Cortiella, A., Doostan, A., Darve, E., IEEE COMPUTER SOC
  IEEE COMPUTER SOC.2025: 1084-1085
- **Hybrid physics-based and data-driven modeling of vascular bifurcation pressure differences.** *Computers in biology and medicine*
  Rubio, N. L., Pegolotti, L., Pfaller, M. R., Darve, E. F., Marsden, A. L.
  2024; 184: 109420
- **Coincident learning for unsupervised anomaly detection of scientific instruments** *MACHINE LEARNING-SCIENCE AND TECHNOLOGY*
  Humble, R., Zhang, Z., OShea, F., Darve, E., Ratner, D.
  2024; 5 (3)
- **A NUMERICALLY STABLE COMMUNICATION-AVOIDING s- STEP GMRES ALGORITHM** *SIAM JOURNAL ON MATRIX ANALYSIS AND APPLICATIONS*
  Xu, Z., Alonso, J., Darve, E.
  2024; 45 (4): 2039-2074
- **Matrix Sketching for Online Analysis of LCLS Imaging Datasets**
  Winnicki, J., Poitevin, F., Li, H., Darve, E., ASSOC COMPUTING MACHINERY
  IEEE.2024: 2144-2153
- **Resilient VAE: Unsupervised Anomaly Detection at the SLAC Linac Coherent Light Source**
  Humble, R., Colocho, W., O'Shea, F., Ratner, D., Darve, E.
  edited by Espinal, DeVita, R., Laycock, P., Shadura, O.
  E D P SCIENCES.2024
- **Learning reduced-order models for cardiovascular simulations with graph neural networks.** *Computers in biology and medicine*
  Pegolotti, L., Pfaller, M. R., Rubio, N. L., Ding, K., Brugarolas Brufau, R., Darve, E., Marsden, A. L.
  2023; 168: 107676
- **Temperature field optimization for laser powder bed fusion as a traveling salesperson problem with history** *INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN ENGINEERING*
  Wang, G., Darve, E., Lew, A. J.
  2023
- **Probabilistic partition of unity networks for high-dimensional regression problems** *INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN ENGINEERING*
  Fan, T., Trask, N., D'Elia, M., Darve, E.
  2023
- **Beam-based rf station fault identification at the SLAC Linac Coherent Light Source** *PHYSICAL REVIEW ACCELERATORS AND BEAMS*
  Humble, R., O'Shea, F. H., Colocho, W., Gibbs, M., Chaffee, H., Darve, E., Ratner, D.
  2022; 25 (12)
- **Variational encoder geostatistical analysis (VEGAS) with an application to large scale riverine bathymetry** *ADVANCES IN WATER RESOURCES*
  Forghani, M., Qian, Y., Lee, J., Farthing, M., Hesser, T., Kitanidis, P. K., Darve, E. F.
  2022; 170
- **HyKKT: a hybrid direct-iterative method for solving KKT linear systems** *OPTIMIZATION METHODS & SOFTWARE*
  Regev, S., Chiang, N., Darve, E., Petra, C. G., Saunders, M. A., Swirydowicz, K., Peles, S.
  2022

- **Second-order accurate hierarchical approximate factorizations for solving sparse linear systems** *INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN ENGINEERING*
  Klockiewicz, B., Cambier, L., Humble, R., Tchelepi, H., Darve, E.
  2022
- **Linear solvers for power grid optimization problems: A review of GPU-accelerated linear solvers** *PARALLEL COMPUTING*
  Swirydowicz, K., Darve, E., Jones, W., Maack, J., Regev, S., Saunders, M. A., Thomas, S. J., Peles, S.
  2022; 111
- **Learning generative neural networks with physics knowledge** *RESEARCH IN THE MATHEMATICAL SCIENCES*
  Xu, K., Zhu, W., Darve, E.
  2022; 9 (2)
- **Hierarchical Orthogonal Factorization: Sparse Least Squares Problems** *JOURNAL OF SCIENTIFIC COMPUTING*
  Gnanasekaran, A., Darve, E.
  2022; 91 (2)
- **Physics constrained learning for data-driven inverse modeling from sparse observations** *JOURNAL OF COMPUTATIONAL PHYSICS*
  Xu, K., Darve, E.
  2022; 453
- **On the fractional Laplacian of variable order** *FRACTIONAL CALCULUS AND APPLIED ANALYSIS*
  Darve, E., D'Elia, M., Garrappa, R., Giusti, A., Rubio, N. L.
  2022; 25 (1): 15-28
- **Integrating deep neural networks with full-waveform inversion: Reparameterization, regularization, and uncertainty quantification** *GEOPHYSICS*
  Zhu, W., Xu, K., Darve, E., Biondi, B., Beroza, G. C.
  2022; 87 (1): R93-R109
- **Soft Masking for Cost-Constrained Channel Pruning**
  Humble, R., Shen, M., Latorre, J., Darve, E., Alvarez, J.
  edited by Avidan, S., Brostow, G., Cisse, M., Farinella, G. M., Hassner, T.
  SPRINGER INTERNATIONAL PUBLISHING AG.2022: 641-657
- **HIERARCHICAL ORTHOGONAL FACTORIZATION: SPARSE SQUARE MATRICES** *SIAM JOURNAL ON MATRIX ANALYSIS AND APPLICATIONS*
  Gnanasekaran, A., Darve, E.
  2022; 43 (1): 94-123
- **Memory-Augmented Generative Adversarial Networks for Anomaly Detection** *IEEE TRANSACTIONS ON NEURAL NETWORKS AND LEARNING SYSTEMS*
  Yang, Z., Zhang, T., Bozchalooi, I., Darve, E.
  2021
- **Learning viscoelasticity models from indirect data using deep neural networks** *COMPUTER METHODS IN APPLIED MECHANICS AND ENGINEERING*
  Xu, K., Tartakovsky, A. M., Burghardt, J., Darve, E.
  2021; 387
- **Solving inverse problems in stochastic models using deep neural networks and adversarial training** *COMPUTER METHODS IN APPLIED MECHANICS AND ENGINEERING*
  Xu, K., Darve, E.
  2021; 384
- **PBBFMM3D: A parallel black-box algorithm for kernel matrix-vector multiplication** *JOURNAL OF PARALLEL AND DISTRIBUTED COMPUTING*
  Wang, R., Chen, C., Lee, J., Darve, E.
  2021; 154: 64-73

- **A general approach to seismic inversion with automatic differentiation** *COMPUTERS & GEOSCIENCES*
  Zhu, W., Xu, K., Darve, E., Beroza, G. C.
  2021; 151
- **Learning constitutive relations using symmetric positive definite neural networks** *JOURNAL OF COMPUTATIONAL PHYSICS*
  Xu, K., Huang, D. Z., Darve, E.
  2021; 428
- **Application of deep learning to large scale riverine flow velocity estimation** *STOCHASTIC ENVIRONMENTAL RESEARCH AND RISK ASSESSMENT*
  Forghani, M., Qian, Y., Lee, J., Farthing, M. W., Hesser, T., Kitanidis, P. K., Darve, E. F.
  2021
- **Deep learning technique for fast inference of large-scale riverine bathymetry** *ADVANCES IN WATER RESOURCES*
  Ghorbanidehno, H., Lee, J., Farthing, M., Hesser, T., Darve, E. F., Kitanidis, P. K.
  2021; 147
- **Universal Sentence Representation Learning with Conditional Masked Language Model**
  Yang, Z., Yang, Y., Cer, D., Law, J., Darve, E., Assoc Computat Linguist
  ASSOC COMPUTATIONAL LINGUISTICS-ACL.2021: 6216-6228
- **A Task-Based Distributed Parallel Sparsified Nested Dissection Algorithm**
  Cambier, L., Darve, E., ACM
  ASSOC COMPUTING MACHINERY.2021
- **A Simple and Effective Method To Eliminate the Self Language Bias in Multilingual Representations**
  Yang, Z., Yang, Y., Cer, D., Darve, E., Assoc Computat Linguist
  ASSOC COMPUTATIONAL LINGUISTICS-ACL.2021: 5825-5832
- **Recent developments in fast and scalable inverse modeling and data assimilation methods in hydrology** *JOURNAL OF HYDROLOGY*
  Ghorbanidehno, H., Kokkinaki, A., Lee, J., Darve, E.
  2020; 591
- **Learning constitutive relations from indirect observations using deep neural networks** *JOURNAL OF COMPUTATIONAL PHYSICS*
  Huang, D. Z., Xu, K., Farhat, C., Darve, E.
  2020; 416
- **Coupled Time-Lapse Full-Waveform Inversion for Subsurface Flow Problems Using Intrusive Automatic Differentiation** *WATER RESOURCES RESEARCH*
  Li, D., Xu, K., Harris, J. M., Darve, E.
  2020; 56 (8)
- **Isogeometric collocation method for the fractional Laplacian in the 2D bounded domain** *COMPUTER METHODS IN APPLIED MECHANICS AND ENGINEERING*
  Xu, K., Darve, E.
  2020; 364
- **Parallelization of the inverse fast multipole method with an application to boundary element method** *COMPUTER PHYSICS COMMUNICATIONS*
  Takahashi, T., Chen, C., Darve, E.
  2020; 247
- **AN ALGEBRAIC SPARSIFIED NESTED DISSECTION ALGORITHM USING LOW-RANK APPROXIMATIONS** *SIAM JOURNAL ON MATRIX ANALYSIS AND APPLICATIONS*
  Cambier, L., Chen, C., Boman, E. G., Rajamanickam, S., Tuminaro, R. S., Darve, E.
  2020; 41 (2): 715–46
- **Regularized Cycle Consistent Generative Adversarial Network for Anomaly Detection**
  Yang, Z., Bozchalooi, I., Darve, E.
  edited by DeGiacomo, G., Catala, A., Dilkina, B., Milano, M., Barro, S., Bugarin, A., Lang, J.

IOS PRESS.2020: 1618-1625

- **TaskTorrent: a Lightweight Distributed Task-Based Runtime System in C plus**
  Cambier, L., Qian, Y., Darve, E., IEEE Comp Soc
  IEEE COMPUTER SOC.2020: 16-26
- **SPARSE HIERARCHICAL PRECONDITIONERS USING PIECEWISE SMOOTH APPROXIMATIONS OF EIGENVECTORS** *SIAM JOURNAL ON SCIENTIFIC COMPUTING*
  Klockiewicz, B., Darve, E.
  2020; 42 (6): A3907–A3931
- **A robust hierarchical solver for ill-conditioned systems with applications to ice sheet modeling** *JOURNAL OF COMPUTATIONAL PHYSICS*
  Chen, C., Cambier, L., Boman, E. G., Rajamanickam, S., Tuminaro, R. S., Darve, E.
  2019; 396: 819–36
- **Sparse hierarchical solvers with guaranteed convergence** *INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN ENGINEERING*
  Yang, K., Pouransari, H., Darve, E.
  2019
- **Erratum: "Investigating the role of non-covalent interactions in conformation and assembly of triazine-based sequence-defined polymers" [J. Chem. Phys. 149, 072330 (2018)].** *The Journal of chemical physics*
  Ahn, S., Grate, J. W., Darve, E. F.
  2019; 150 (17): 179901
- **The multi-dimensional generalized Langevin equation for conformational motion of proteins** *JOURNAL OF CHEMICAL PHYSICS*
  Lee, H., Ahn, S., Darve, E. F.
  2019; 150 (17)
- **The multi-dimensional generalized Langevin equation for conformational motion of proteins** *JOURNAL OF CHEMICAL PHYSICS*
  Lee, H., Ahn, S., Darve, E. F.
  2019; 150 (17)
- **Novel Data Assimilation Algorithm for Nearshore Bathymetry** *JOURNAL OF ATMOSPHERIC AND OCEANIC TECHNOLOGY*
  Ghorbanidehno, H., Lee, J., Farthing, M., Hesser, T., Kitanidis, P. K., Darve, E. F.
  2019; 36 (4): 699–715
- **The multi-dimensional generalized Langevin equation for conformational motion of proteins.** *The Journal of chemical physics*
  Lee, H. S., Ahn, S. H., Darve, E. F.
  2019; 150 (17): 174113
- **Embedding Imputation with Grounded Language Information**
  Yang, Z., Zhu, C., Sachidananda, V., Darve, E., ACL
  edited by Korhonen, A., Traum, D., Marquez, L.
  ASSOC COMPUTATIONAL LINGUISTICS-ACL.2019: 3356–61
- **BLOCK BASIS FACTORIZATION FOR SCALABLE KERNEL EVALUATION** *SIAM JOURNAL ON MATRIX ANALYSIS AND APPLICATIONS*
  Wang, R., Li, Y., Mahoney, M. W., Darve, E.
  2019; 40 (4): 1497–1526
- **FAST LOW-RANK KERNEL MATRIX FACTORIZATION USING SKELETONIZED INTERPOLATION** *SIAM JOURNAL ON SCIENTIFIC COMPUTING*
  Cambier, L., Darve, E.
  2019; 41 (3): A1652–A1680
- **Investigating the role of non-covalent interactions in conformation and assembly of triazine-based sequence-defined polymers.** *The Journal of chemical physics*
  Ahn, S., Grate, J. W., Darve, E. F.
  2018; 149 (7): 072330
- **Sparse supernodal solver using block low-rank compression: Design, performance and analysis** *JOURNAL OF COMPUTATIONAL SCIENCE*
  Pichon, G., Darve, E., Faverge, M., Ramet, P., Roman, J.

2018; 27: 255–70

- **A distributed-memory hierarchical solver for general sparse linear systems**
  Chen, C., Pouransari, H., Rajamanickam, S., Boman, E. G., Darve, E.
  ELSEVIER SCIENCE BV.2018: 49–64

- **Riverine Bathymetry Imaging With Indirect Observations** *WATER RESOURCES RESEARCH*
  Lee, J., Ghorbanidehno, H., Farthing, M. W., Hesser, T. J., Darve, E. F., Kitanidis, P. K.
  2018; 54 (5): 3704–27

- **An efficient preconditioner for the fast simulation of a 2D stokes flow in porous media** *INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN ENGINEERING*
  Quaife, B., Coulier, P., Darve, E.
  2018; 113 (4): 561–80

- **ON THE NUMERICAL RANK OF RADIAL BASIS FUNCTION KERNELS IN HIGH DIMENSIONS** *SIAM JOURNAL ON MATRIX ANALYSIS AND APPLICATIONS*
  Wang, R., Li, Y., Darve, E.
  2018; 39 (4): 1810–35

- **LOW-RANK FACTORIZATIONS IN DATA SPARSE HIERARCHICAL ALGORITHMS FOR PRECONDITIONING SYMMETRIC POSITIVE DEFINITE MATRICES** *SIAM JOURNAL ON MATRIX ANALYSIS AND APPLICATIONS*
  Agullo, E., Darve, E., Giraud, L., Harness, Y.
  2018; 39 (4): 1701–25

- **Optimal estimation and scheduling in aquifer management using the rapid feedback control method** *ADVANCES IN WATER RESOURCES*
  Ghorbanidehno, H., Kokkinaki, A., Kitanidis, P. K., Darve, E.
  2017; 110: 310–18

- **Efficiently sampling conformations and pathways using the concurrent adaptive sampling (CAS) algorithm.** *The Journal of chemical physics*
  Ahn, S. H., Grate, J. W., Darve, E. F.
  2017; 147 (7): 074115

- **Smoothing-based compressed state Kalman filter for joint state-parameter estimation: Applications in reservoir characterization and CO2 storage monitoring** *WATER RESOURCES RESEARCH*
  Li, Y. J., Kokkinaki, A., Darve, E. F., Kitanidis, P. K.
  2017; 53 (8): 7190–7207

- **A numerical study of super-resolution through fast 3D wideband algorithm for scattering in highly-heterogeneous media** *WAVE MOTION*
  Letourneau, P., Wu, Y., Papanicolaou, G., Garnier, J., Darve, E.
  2017; 70: 113-134

- **Computing the non-Markovian coarse-grained interactions derived from the Mori-Zwanzig formalism in molecular systems: Application to polymer melts** *JOURNAL OF CHEMICAL PHYSICS*
  Li, Z., Lee, H. S., Darve, E., Karniadakis, G. E.
  2017; 146 (1)

- **Sparse Supernodal Solver Using Block Low-Rank Compression**
  Pichon, G., Darve, E., Faverge, M., Ramet, P., Roman, J., IEEE
  IEEE.2017: 1138–47

- **Efficient mesh deformation based on radial basis function interpolation by means of the inverse fast multipole method** *COMPUTER METHODS IN APPLIED MECHANICS AND ENGINEERING*
  Coulier, P., Darve, E.
  2016; 308: 286-309

- **A fast, memory efficient and robust sparse preconditioner based on a multifrontal approach with applications to finite-element matrices** *INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN ENGINEERING*
  Aminfar, A., Darve, E.
  2016; 107 (6): 520-540

- **Task-based FMM for heterogeneous architectures** *CONCURRENCY AND COMPUTATION-PRACTICE & EXPERIENCE*
  Agullo, E., Bramas, B., Coulaud, O., Darve, E., Messner, M., Takahashi, T.
  2016; 28 (9): 2608-2629
- **A fast block low-rank dense solver with applications to finite-element matrices** *JOURNAL OF COMPUTATIONAL PHYSICS*
  Aminfar, A., Ambikasaran, S., Darve, E.
  2016; 304: 170-188
- **Real-time data assimilation for large-scale systems: The spectral Kalman filter** *ADVANCES IN WATER RESOURCES*
  Ghorbanidehno, H., Kokkinaki, A., Li, J. Y., Darve, E., Kitanidis, P. K.
  2015; 86: 260-272
- **The compressed state Kalman filter for nonlinear state estimation: Application to large-scale reservoir monitoring** *WATER RESOURCES RESEARCH*
  Li, J. Y., Kokkinaki, A., Ghorbanidehno, H., Darve, E. F., Kitanidis, P. K.
  2015; 51 (12): 9942-9963
- **A new sparse matrix vector multiplication graphics processing unit algorithm designed for finite element problems** *INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN ENGINEERING*
  Wong, J., Kuhl, E., Darve, E.
  2015; 102 (12): 1784-1814
- **A comparison of weighted ensemble and Markov state model methodologies** *JOURNAL OF CHEMICAL PHYSICS*
  Feng, H., Costaouec, R., Darve, E., Izaguirre, J. A.
  2015; 142 (21)
- **OPTIMIZING THE ADAPTIVE FAST MULTIPOLE METHOD FOR FRACTAL SETS** *SIAM JOURNAL ON SCIENTIFIC COMPUTING*
  Pouransari, H., Darve, E.
  2015; 37 (2): A1040-A1066
- **AWE-WQ: Fast-Forwarding Molecular Dynamics Using the Accelerated Weighted Ensemble** *JOURNAL OF CHEMICAL INFORMATION AND MODELING*
  Abdul-Wahid, B., Feng, H., Rajan, D., Costaouec, R., Darve, E., Thain, D., Izaguirre, J. A.
  2014; 54 (10): 3033-3043
- **A Kalman filter powered by H-2-matrices for quasi-continuous data assimilation problems** *WATER RESOURCES RESEARCH*
  Li, J. Y., Ambikasaran, S., Darve, E. F., Kitanidis, P. K.
  2014; 50 (5): 3734-3749
- **Method and advantages of genetic algorithms in parameterization of interatomic potentials: Metal oxides** *COMPUTATIONAL MATERIALS SCIENCE*
  Solomon, J., Chung, P., Srivastava, D., Darve, E.
  2014; 81: 453-465
- **CAUCHY FAST MULTIPOLE METHOD FOR GENERAL ANALYTIC KERNELS** *SIAM JOURNAL ON SCIENTIFIC COMPUTING*
  Letourneau, P., Cecka, C., Darve, E.
  2014; 36 (2): A396-A426
- **TASK-BASED FMM FOR MULTICORE ARCHITECTURES** *SIAM JOURNAL ON SCIENTIFIC COMPUTING*
  Agullo, E., Bramas, B., Coulaud, O., Darve, E., Messner, M., Takahashi, T.
  2014; 36 (1): C66-C93
- **An Fast Direct Solver for Partial Hierarchically Semi-Separable Matrices** *JOURNAL OF SCIENTIFIC COMPUTING*
  Ambikasaran, S., Darve, E.
  2013; 57 (3): 477-501
- **Large-scale stochastic linear inversion using hierarchical matrices** *COMPUTATIONAL GEOSCIENCES*
  Ambikasaran, S., Li, J. Y., Kitanidis, P. K., Darve, E.
  2013; 17 (6): 913-927

- **ANALYSIS OF THE ACCELERATED WEIGHTED ENSEMBLE METHODOLOGY** *DISCRETE AND CONTINUOUS DYNAMICAL SYSTEMS*
  Costaouec, R., Feng, H., Izaguirre, J., Darve, E.
  2013: 171-181
- **The accuracy of the CHARMM22/CMAP and AMBER ff99SB force fields for modelling the antimicrobial peptide cecropin P1** *MOLECULAR SIMULATION*
  Kia, A., Darve, E.
  2013; 39 (11): 922-936
- **A fast algorithm for sparse matrix computations related to inversion** *JOURNAL OF COMPUTATIONAL PHYSICS*
  Li, S., Wu, W., Darve, E.
  2013; 242: 915-945
- **FOURIER-BASED FAST MULTIPOLE METHOD FOR THE HELMHOLTZ EQUATION** *SIAM JOURNAL ON SCIENTIFIC COMPUTING*
  Cecka, C., Darve, E.
  2013; 35 (1): A79-A103
- **Accuracy in One-way and Two-way Algorithms for Computing Desired Entries in the Inverse of Sparse Matrices** *11th International Conference of Numerical Analysis and Applied Mathematics (ICNAAM)*
  Li, S., Darve, E.
  AMER INST PHYSICS.2013: 1501–1504
- **Task-based FMM for multicore architectures**
  Agullo, E., Bramas, B., Coulaud, O., Darve, E., Messner, M., Takahashi, T.
  2013
- **An\ mathcal O (N\ log N) Fast Direct Solver for Partial Hierarchically Semi-Separable Matrices** *Journal of Scientific Computing*
  Ambikasaran, S., Darve, E.
  2013; 57 (3): 477-501
- **Fast Algorithms for Bayesian Inversion** *Computational Challenges in the Geosciences*
  Ambikasaran, S., Saibaba, A. K., Darve, E. F., Kitanidis, Peter, K.
  2013; 156: 101-142
- **Task-based Parallelization of the Fast Multipole Method on NVIDIA GPUs and Multicore Processors**
  Agullo, E., Bramas, B., Coulaud, O., Darve, E., Messner, M., Takahashi, T.
  2013
- **Optimizing the Black-box FMM for Smooth and Oscillatory Kernels**
  Darve, E., Messner, M., Schanz, M., Coulaud, O.
  2013
- **Composition and reuse with compiled domain-specific languages**
  Darve, E., Sujeeth, Arvind, K., Rompf, T., Brown, Kevin, J., Lee, H., Chafi, H.
  2013
- **Folding Proteins at 500 ns/hour with Work Queue.** *Proceedings ... IEEE International Conference on eScience. IEEE International Conference on eScience*
  Abdul-Wahid, B., Yu, L., Rajan, D., Feng, H., Darve, E., Thain, D., Izaguirre, J. A.
  2012; 2012: 1-8
- **Application of Hierarchical Matrices to Linear Inverse Problems in Geostatistics** *OIL & GAS SCIENCE AND TECHNOLOGY-REVUE D IFP ENERGIES NOUVELLES*
  Saibaba, A. K., Ambikasaran, S., Li, J. Y., Kitanidis, P. K., Darve, E. F.
  2012; 67 (5): 857-875
- **Fast directional multilevel summation for oscillatory kernels based on Chebyshev interpolation** *JOURNAL OF COMPUTATIONAL PHYSICS*
  Messner, M., Schanz, M., Darve, E.
  2012; 231 (4): 1175-1196

- **Extension and optimization of the FIND algorithm: Computing Green's and less-than Green's functions** *JOURNAL OF COMPUTATIONAL PHYSICS*
  Li, S., Darve, E.
  2012; 231 (4): 1121-1139
- **Optimizing the multipole-to-local operator in the fast multipole method for graphical processing units** *INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN ENGINEERING*
  Takahashi, T., Cecka, C., Fong, W., Darve, E.
  2012; 89 (1): 105-133
- **Time integrators based on approximate discontinuous Hamiltonians** *INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN ENGINEERING*
  Dharmaraja, S., Kesari, H., Darve, E., Lew, A. J.
  2012; 89 (1): 71-104
- **Fast Multipole Method Using the Cauchy Integral Formula** *Workshop on Numerical Analysis and Multiscale Computations*
  Cecka, C., Letourneau, P., Darve, E.
  SPRINGER-VERLAG BERLIN.2012: 127–144
- **Folding Proteins at 500 ns/hour with Work Queue** *IEEE 8th International Conference on E-Science (e-Science)*
  Abdul-Wahid, B., Yu, L., Rajan, D., Feng, H., Darve, E., Thain, D., Izaguirre, J. A.
  IEEE.2012
- **Optimization of the parallel black-box fast multipole method on CUDA** *Innovative Parallel Computing (InPar)*
  Takahashi, T., Cecka, C., Darve, E.
  2012: 1 - 14
- **Poster: Matrices over Runtime Systems at Exascale**
  Darve, E., Agullo, E., Bosilca, G., Bramas, B., Castagnede, C., Coulaud, O.
  2012
- **Folding Proteins at 500 ns/hour with Work Queue**
  Abdul-Wahid, B., Yu, L., Rajan, D., Feng, H., Darve, E., Thain, D.
  2012
- **EFFICIENT DATA ASSIMILATION TOOL IN CONJUNCTION WITH TOUGH2 FOR CO2 MONITORING**
  Li, J. Y., Ambikasaran, S., Kitanidis, P. K., Darve, E.
  2012
- **Matrices Over Runtime Systems at Exascale**
  Agullo, E., Bosilca, G., Bramas, B., Castagnede, C., Coulaud, O., Darve, E.
  2012
- **Matrices Over Runtime Systems @ Exascale** *25th ACM/IEEE International Conference for High Performance Computing, Networking, Storage and Analysis (SC)*
  Agullo, E., Bosilca, G., Bramas, B., Castagnede, C., Coulaud, O., Darve, E., Dongarra, J., Faverge, M., Furmento, N., Giraud, L., Lacoste, X., Langou, J., Ltaief, et al
  IEEE.2012: 1330–1331
- **Assembly of finite element methods on graphics processors** *INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN ENGINEERING*
  Cecka, C., Lew, A. J., Darve, E.
  2011; 85 (5): 640-669
- **The fast multipole method on parallel clusters, multicore processors, and graphics processing units** *COMPTES RENDUS MECANIQUE*
  Darve, E., Cecka, C., Takahashi, T.
  2011; 339 (2-3): 185-193
- **Liszt: a domain specific language for building portable mesh-based PDE solvers**
  DeVito, Z., Joubert, N., Palacios, F., Oakley, S., Medina, M., Barrientos, M., Darve, E.
  2011

- **Generalized Fast Multipole Method** *9th World Congress on Computational Mechanics/4th Asian Pacific Congress on Computational Mechanics*
  Letourneau, P., Cecka, C., Darve, E.
  IOP PUBLISHING LTD.2010
- **The CUDA codes to perform M2L operation in FMM**
  Takahashi, T., Cecka, C., Fong, W., Darve, E.
  2010
- **Generalized fast multipole method**
  Létourneau, P. D., Cecka, C., Darve, E.
  2010
- **An implementation of low-frequency fast multipole BIEM for Helmholtz'equation on GPU**
  Takahashi, T., Cecka, C., Darve, E.
  2010
- **Application of assembly of finite element methods on graphics processors for real-time elastodynamics** *GPU Computing Gems*
  Cecka, C., Lew, A., Darve, E.
  edited by Hwu, Wen-mei, W.
  Elsevier.2010: 1
- **Introduction to Assembly of Finite Element Methods on Graphics Processors** *9th World Congress on Computational Mechanics/4th Asian Pacific Congress on Computational Mechanics*
  Cecka, C., Lew, A., Darve, E.
  IOP PUBLISHING LTD.2010
- **The black-box fast multipole method** *JOURNAL OF COMPUTATIONAL PHYSICS*
  Fong, W., Darve, E.
  2009; 228 (23): 8712-8725
- **A hybrid method for the parallel computation of Green's functions** *JOURNAL OF COMPUTATIONAL PHYSICS*
  Petersen, D. E., Li, S., Stokbro, K., Sorensen, H. H., Hansen, P. C., Skelboe, S., Darve, E.
  2009; 228 (14): 5020-5039
- **Computing generalized Langevin equations and generalized Fokker-Planck equations** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
  Darve, E., Solomon, J., Kia, A.
  2009; 106 (27): 10884-10889
- **High-ionic-strength electroosmotic flows in uncharged hydrophobic nanochannels** *JOURNAL OF COLLOID AND INTERFACE SCIENCE*
  Kim, D., Darve, E.
  2009; 330 (1): 194-200
- **Optimization of the FIND Algorithm to Compute the Inverse of a Sparse Matrix** *13th International Workshop on Computational Electronics*
  Li, S., Darve, E.
  IEEE.2009: 285–288
- **Concentration distributions of arbitrary shaped particles in microfluidic channel flows** *Bulletin of the American Physical Society*
  Saibaba, A., Shaqfeh, E., Darve, E.
  2009; 54 (19)
- **Optimization of the FIND algorithm to compute the inverse of a sparse matrix**
  Li, S., Darve, E.
  2009
- **Computing generalized Langevin equations and generalized Fokker–Planck equations**
  Darve, E., Solomon, J., Kia, A.
  edited by Chorin, Alexandre, J.
  2009

- **Large calculation of the flow over a hypersonic vehicle using a GPU** *JOURNAL OF COMPUTATIONAL PHYSICS*
  Elsen, E., LeGresley, P., Darve, E.
  2008; 227 (24): 10148-10161
- **Computing entries of the inverse of a sparse matrix using the FIND algorithm** *JOURNAL OF COMPUTATIONAL PHYSICS*
  Li, S., Ahmed, S., Klimeck, G., Darve, E.
  2008; 227 (22): 9408-9427
- **Fast electrostatic force calculation on parallel computer clusters** *JOURNAL OF COMPUTATIONAL PHYSICS*
  Kia, A., Kim, D., Darve, E.
  2008; 227 (19): 8551-8567
- **Stability of asynchronous variational integrators** *JOURNAL OF COMPUTATIONAL PHYSICS*
  Fong, W., Darve, E., Lew, A.
  2008; 227 (18): 8367-8394
- **Adaptive biasing force method for scalar and vector free energy calculations** *JOURNAL OF CHEMICAL PHYSICS*
  Darve, E., Rodriguez-Gomez, D., Pohorille, A.
  2008; 128 (14)
- **A black-box Fast Multipole Method**
  Darve, E., Fong, W.
  2008
- **BIRS 08w5074: Mathematical and numerical methods for free energy calculations in molecular systems**
  Darve, E., Chipot, C.
  2008
- **Fast inverse using nested dissection for NEGF** *JOURNAL OF COMPUTATIONAL ELECTRONICS*
  Li, S., Ahmed, S., Darve, E.
  2007; 6 (1-3): 187-190
- **Stability of asynchronous variational integrators** *21st International Workshop on Principles of Advanced and Distributed Simulation (PADS 2007)*
  Fong, W., Darve, E., Lew, A.
  IEEE COMPUTER SOC.2007: 38–44
- **Thermodynamic integration using constrained and unconstrained dynamics** *Free Energy Calculations*
  Darve, E.
  2007; 86: 119-170
- **The effect of stratification on the wave number selection in the instability of sedimenting spheroids** *PHYSICS OF FLUIDS*
  Saintillan, D., Shaqfeh, E. S., Darve, E.
  2006; 18 (12)
- **Stabilization of a suspension of sedimenting rods by induced-charge electrophoresis** *PHYSICS OF FLUIDS*
  Saintillan, D., Shaqfeh, E. S., Darve, E.
  2006; 18 (12)
- **Hydrodynamic interactions in the induced-charge electrophoresis of colloidal rod dispersions** *JOURNAL OF FLUID MECHANICS*
  Saintillan, D., Darve, E., Shaqfeh, E. S.
  2006; 563: 223-259
- **Effect of flexibility on the shear-induced migration of short-chain polymers in parabolic channel flow** *JOURNAL OF FLUID MECHANICS*
  Saintillan, D., Shaqfeh, E. S., Darve, E.
  2006; 557: 297-306
- **Molecular dynamics simulation of electro-osmotic flows in rough wall nanochannels** *PHYSICAL REVIEW E*
  Kim, D., Darve, E.
  2006; 73 (5)

- **The growth of concentration fluctuations in dilute dispersions of orientable and deformable particles under sedimentation** *JOURNAL OF FLUID MECHANICS*
  Saintillan, D., Shaqfeh, E. S., Darve, E.
  2006; 553: 347-388
- **Numerical Methods for Calculating the Potential of Mean Force** *New Algorithms for Macromolecular Simulation*
  Darve, E.
  2006; 49: 213-249
- **Stratification and wavenumber selection in the instability of sedimenting spheroids**
  Saintillan, D., Shaqfeh, E. S., Darve, E.
  2006
- **The Dynamics of Rodlike Particles under Sedimentation and Induced-Charge Electrophoresis**
  Shaqfeh, E. S., Saintillan, D., Darve, E.
  2006
- **Adaptive Biasing Force Method for Vector Free Energy Calculations**
  Darve, E.
  2006
- **Electric Double Layer Structures near Rough Surfaces: Molecular Dynamics Simulation** *Bulletin of the American Physical Society*
  Kim, D., Darve, E.
  2006
- **Fast Inverse using Nested Dissection for the Non Equilibrium Green's Function** *11th International Workshop on Computational Electronics*
  Li, S., Darve, E.
  2006
- **Effect of flexibility on the shear-induced migration of short polymers in parabolic channel flow**
  Saintillan, D., Shaqfeh, E. S., Darve, E.
  2006
- **Effect of flexibility on the shear-induced migration of short polymers in parabolic channel flow**
  Saintillan, D., Shaqfeh, E. S., Darve, E.
  2006
- **A smooth particle-mesh Ewald algorithm for Stokes suspension simulations: The sedimentation of fibers** *PHYSICS OF FLUIDS*
  Saintillan, D., Darve, E., Shaqfeh, E. S.
  2005; 17 (3)
- **Interactions of wall roughness and electroosmotic flows inside nanochannels** *3rd International Conference on Microchannels and Minichannels*
  Kim, D., Darve, E.
  AMER SOC MECHANICAL ENGINEERS.2005: 641–645
- **Concentration fluctuations in dilute suspensions of orientable and deformable particles under sedimentation**
  Saintillan, D., Shaqfeh, E. S., Darve, E.
  2005
- **Hydrodynamic interactions in colloidal dispersions of conducting rods under induced-charge electrophoresis**
  Saintillan, D., Shaqfeh, E. S., Darve, E.
  2005
- **Induced-charge electrophoresis in suspensions of rodlike particles: Theory and simulations** *ASME International Mechanical Engineering Congress and Exposition*
  Saintillan, D., Darve, E., Shaqfeh, E. S.
  AMER SOC MECHANICAL ENGINEERS.2005: 251–256
- **Microstructure in the sedimentation of anisotropic and deformable particles** *ASME International Mechanical Engineering Congress and Exposition*

Saintillan, D., Darve, E., Shaqfeh, E. S.
AMER SOC MECHANICAL ENGINEERS.2005: 797–803

- **Efficient fast multipole method for low-frequency scattering** *JOURNAL OF COMPUTATIONAL PHYSICS*
  Darve, E., Have, P.
  2004; 197 (1): 341-363
- **A fast multipole method for Maxwell equations stable at all frequencies** *PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A-MATHEMATICAL PHYSICAL AND ENGINEERING SCIENCES*
  Darve, E., Have, P.
  2004; 362 (1816): 603-628
- **Assessing the efficiency of free energy calculation methods** *JOURNAL OF CHEMICAL PHYSICS*
  Rodriguez-Gomez, D., Darve, E., Pohorille, A.
  2004; 120 (8): 3563-3578
- **Calculating transport properties of nanodevices** *Conference on Nanosensing*
  Darve, E., Li, S., Teslyar, Y.
  SPIE-INT SOC OPTICAL ENGINEERING.2004: 452–463
- **Computing flow rate of electroosmotic flows in nanochannels with different wall roughness** *The Smithsonian/NASA Astrophysics Data System*
  Kim, D., Darve, E.
  2004
- **Calculating transport properties of nanodevices**
  Darve, E. F., Li, S., Teslyar, Y.
  2004
- **Dynamic Simulations of Sedimenting Fibers with Fast Fourier Transform Acceleration** *Abstracts of the Papers*
  Darve, E., Saintillan, D., Shaqfeh, E. S.
  2004
- **Pattern formation in sedimenting suspensions of spheroids**
  Saintillan, D., Darve, E., Shaqfeh, E. S.
  2004
- **Analysis and performance results of a molecular modeling application on Merrimac**
  Erez, M., Ahn, J. H., Garg, A., Dally, W. J., Darve, E.
  2004
- **Fast multipole method for low-frequency electromagnetic scattering** *2nd MIT Conference on Computational Fluid and Solid Mechanics*
  Darve, E., Have, P.
  ELSEVIER SCIENCE BV.2003: 1299–1302
- **Unfolding of proteins: Thermal and mechanical unfolding**
  Hur, J. S., Darve, E.
  2003
- **Surface tension evaluation in lennard-jones fluid system with untruncated potentials**
  Sinha, S., Shi, B., Dhir, Vijay, K., Freund, Jonathan, B., Darve, E.
  2003
- **Calculating free energies using a scaled-force molecular dynamics algorithm** *MOLECULAR SIMULATION*
  Darve, E., Wilson, M. A., Pohorille, A.
  2002; 28 (1-2): 113-144
- **Calculating free energies using average force** *JOURNAL OF CHEMICAL PHYSICS*
  Darve, E., Pohorille, A.
  2001; 115 (20): 9169-9183

- **The fast multipole method I: error analysis and asymptotic complexity** *SIAM JOURNAL ON NUMERICAL ANALYSIS*
  Darve, E.
  2000; 38 (1): 98-128
- **The fast multipole method: Numerical implementation** *JOURNAL OF COMPUTATIONAL PHYSICS*
  Darve, E.
  2000; 160 (1): 195-240
- **Méthodes multipôles rapides: Résolution des équations de Maxwell par formulations intégrales**
  Darve, E., Olivier, P.
  1999; 133 (99 PA06 6598): 228
- **Advanced structured-unstructured solver for electromagnetic scattering from multimaterial objects**
  Darve, E., Loehner, R.
  1997
- **Fast-multipole method: a mathematical study** *Comptes Rendus de l'Académie des Sciences-Series I-Mathematics*
  Darve, E.
  1997; 325 (9): 1037–1042
- **THE MULTISTEP FAST MULTIPOLE METHOD: ALGORITHM AND ERROR ESTIMATION**
  DARVE, E.
  1997
- **SOLVING THE SCALAR WAVE EQUATION VIA A DIRECTIONAL FAST MULTIPOLE METHOD**
  MESSNER, M., DARVE, E., SCHANZ, M.
- **A KALMAN FILTER POWERED BY H-MATRICES FOR QUASI-CONTINUOUS DATA ASSIMILATION PROBLEMS**
  LI, Y. J., AMBIKASARAN, S., DARVE, E. F., KITANIDIS, P. K.
- **Concentration fluctuations in the dilute sedimentation of anisotropic particles** *15th US National Congress*
  Darve, E., SAINTILLAN, D., SHAQFEH, E. S.
- **CFD for Blood Transfusions on the Battlefield and Inhalation of Toxic Agents in the Lung**
  Shaqfeh, E. E., Iaccarino, G., Darve, E.
- **Dynamic simulations of the instability of sedimenting fibers**
  Saintillan, D., Darve, E., Shaqfeh, E. S.